Appendix VIII: Radiocarbon Dating Report

Radiocarbon Dating Report to the Mother and Baby Homes Commission of Investigation

Author: Professor Gordon T Cook

Date: 3rd November 2016

INTRODUCTION

This report relates to the radiocarbon dating of 6 infant bone samples (see Plates 1-6 below) submitted to the SUERC Radiocarbon Dating Laboratory by Aidan Harte on the 12th October 2016, on behalf of the Mother and Baby Homes Commission of Investigation in Ireland. The remains are from the reported 'Children's Burial Ground' related to St Mary's Mother and Baby Home at Tuam, Co. Galway. This Home operated between 1925 and 1961 and occupied a former Union Workhouse that was operational from around 1846 until 1916. There have been remains discovered associated with this workhouse in previous excavations c.100 m from the current location. However, the remains associated with the workhouse time frame were more formally buried than the 6 samples submitted to the laboratory.

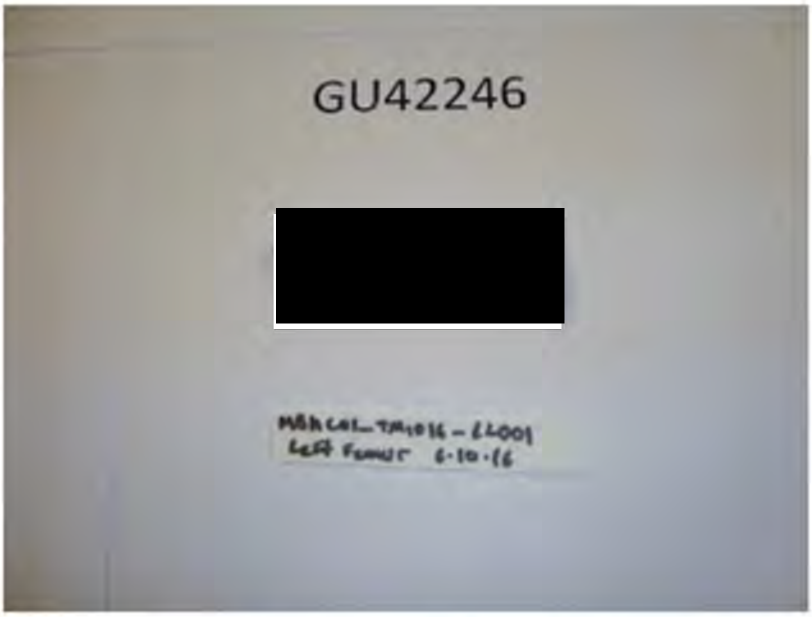


Plate 1: Left femur (Sample LL001) from an infant around 1.5 months of age. Our Laboratory Ref: GU-42246. Our Analysis Ref: SUERC-69881.

Plate 2: Left temporal bone (Sample LL002) from an infant around 0-6 months of age. Our Laboratory Ref: GU-42247. Our Analysis Ref: SUERC-69882.

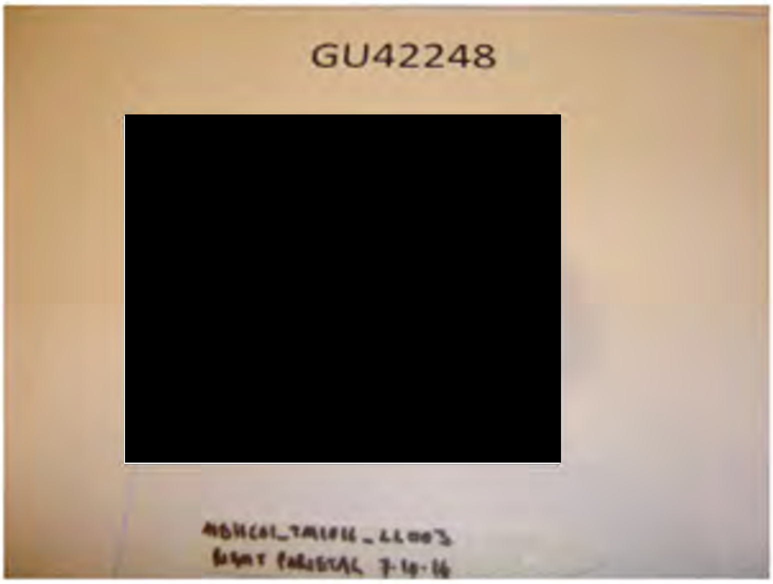


Plate 3: Right parietal bone (Sample LL003) from an infant less than 6 months of age. Our Laboratory Ref: GU-42248. Our Analysis Ref: SUERC-69883.

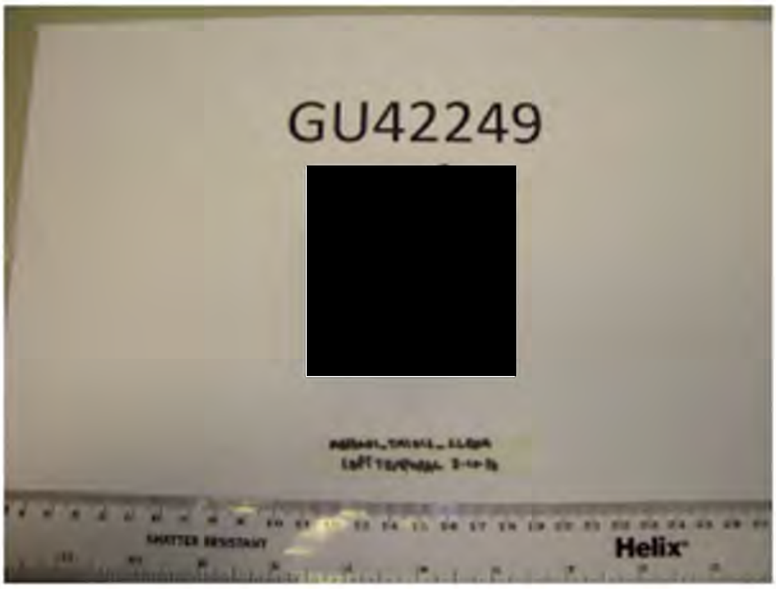


Plate 4: Left temporal bone (Sample LL004) from an infant of between 6 and 12 months age. Our Laboratory Ref: GU-42249. Our Analysis Ref: SUERC-69884.

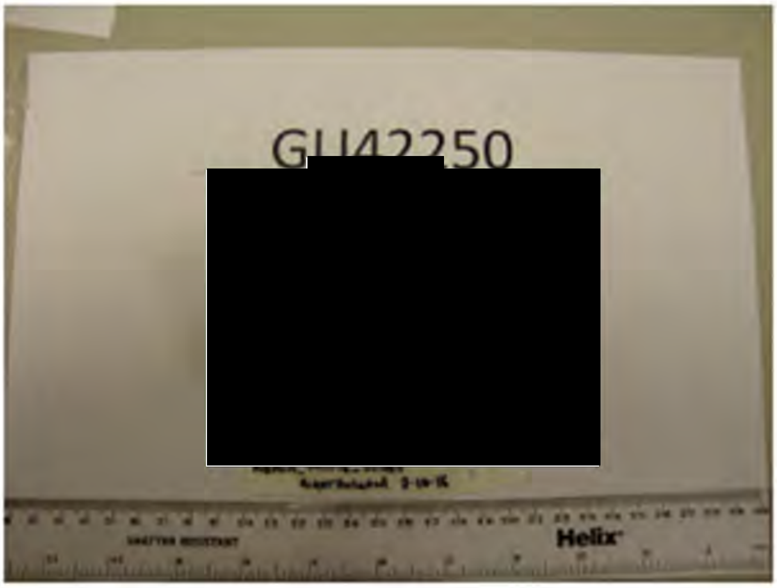


Plate 5: Right parietal bone (Sample LL005) from an infant of between 6 and 12 months age. Our Laboratory Ref: GU-42250. Our Analysis Ref: SUERC-69885.

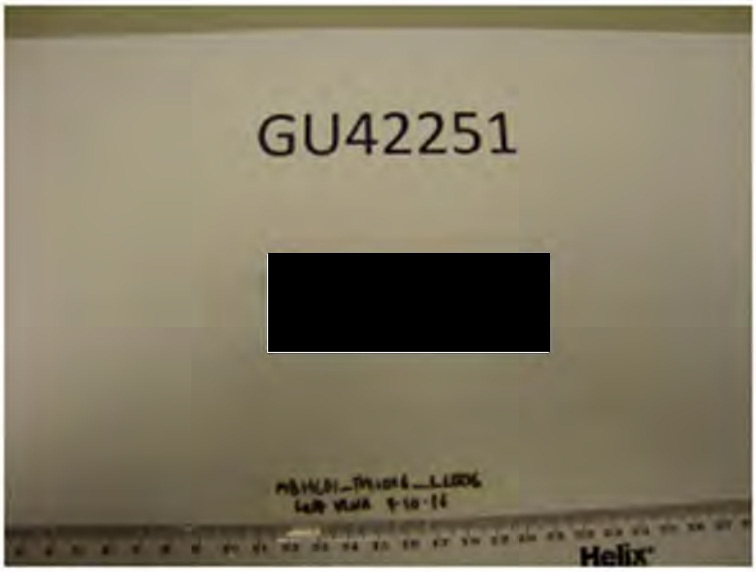


Plate 6: Left ulna (Sample LL006) from an infant of between 3 and 6 months age. Our Laboratory Ref: GU-42251. Our Analysis Ref: SUERC-69886.

BASIC RADIOCARBON PRINCIPLES AND ASSUMPTIONS IN THE METHOD

Radiocarbon, or ^{14}C, is cosmogenic, *i.e.* it is produced as a result of cosmic activity. The primary cosmic radiation is predominantly high energy protons (up to 10^{18} eV), which interact with atmospheric gases producing neutrons, protons, α-particles, *etc.* The neutrons are thermalised and captured by atmospheric nitrogen in the upper atmosphere, resulting in ^{14}C production by the following reaction:

$$^{14}N(n,p)^{14}C$$

^{14}C is radioactive and decays by β^- decay (E_{max} = 156 keV) back to ^{14}N. The physical half-life is 5730 years. The Libby half-life, which is used to calculate radiocarbon ages, is 5568 years. The natural rate of production is not constant, but is subject to short-term (century scale) and long-term (millennia scale) fluctuations. The short-term fluctuations are usually attributed to heliomagnetic modulation of the primary cosmic-ray flux (Stuiver 1961; Damon *et al.* 1989), *i.e.* changes in the solar sunspot activity where periods of high activity result in decreased cosmic ray incidence on the earth and hence a reduced ^{14}C production rate. The longer term fluctuations are attributed to geomagnetic modulation, *i.e.* the charged cosmic rays which create ^{14}C are deflected to a greater or lesser degree depending on the earth's dipole moment (Elsasser *et al.* 1956; Sternberg 1992). The ^{14}C produced in the upper atmosphere is rapidly oxidised to $^{14}CO_2$, which mixes with the stable CO_2 ($^{13}CO_2$ and ^{12}CO), resulting in an atom ratio for the three isotopes of approximately:

$$\begin{array}{ccccc} ^{12}C & : & ^{13}C & : & ^{14}C \\ 10^{12} & : & 10^{10} & : & 1 \end{array}$$

With the onset of the Industrial Revolution came man's first significant perturbation of the natural ^{14}C/stable carbon ratios in the environment. The massive burning of fossil fuels which, because of their age, contain no ^{14}C has resulted in the release of only stable CO_2 to the atmosphere ($^{12}CO_2$ and $^{13}CO_2$), thereby diluting the $^{14}CO_2$ activity (Suess 1953, 1955). This dilution, commonly known as the Suess Effect, was measurable in post-1890AD tree rings and by 1950AD the atmospheric activity was reduced by about 2% and 3% in the southern and northern hemispheres, respectively. The consequence of this from a radiocarbon dating viewpoint is that it is not possible to distinguish between a sample (organism) that died in the 17th century and whose activity has undergone around 300 years of decay and a sample that formed during the period 1890 to 1950 whose activity is influenced by the Suess Effect.

From the early 1950s came the onset of major programmes of atmospheric nuclear weapons testing which caused a significant increase in the atmospheric concentration of ^{14}C such that by 1963 the activity in the northern hemisphere was approximately double the natural level (Figure 1). However, following a test ban treaty, the atmospheric concentration has continuously decreased from around 1963/64 onwards as the excess $^{14}CO_2$ has been taken up by the oceans and the biota.

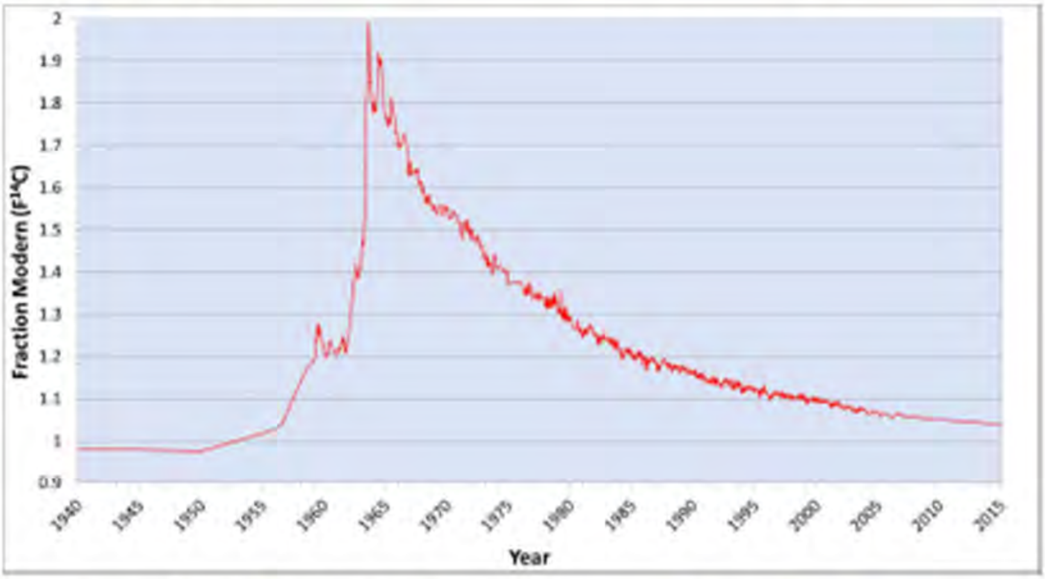


Figure 1: Atmospheric ^{14}C activity in the N Hemisphere during the period 1950–2015

Regardless of the route of formation, ^{14}C becomes incorporated into the food chain via photosynthesis by the primary producers, according to the following reaction.

$$6CO_2 + 6H_2O \xrightarrow[\text{Photosynthetic pigments}]{\text{Light}} C_6H_{12}O_6 + 6O_2$$

Subsequent transfer through the food chain results in radioactive labelling of all living organisms.

$$Plant\ carbohydrates \xrightarrow{Transfer\ through\ food\ chain} Animal\ life$$

N.B. As a consequence of atmospheric nuclear weapons testing, any short-lived sample that has a fraction modern value greater than 1 must have been alive after 1955 (see Figure 1). However, a problem arises when dealing with human bone. The dateable fraction is a protein termed collagen (see below) which, particularly in adults, turns over relatively slowly (Hedges et al. 2007). Consequently, it is not the ^{14}C within bone collagen formed during the year of death that is measured but an integration of collagen from formation and turnover processes over a number of years. Therefore, in the absence of other information, the use of single ^{14}C measurements on bone collagen from juveniles and adults can only provide very limited information, i.e. whether or not the person died during the nuclear era (because their ^{14}C activity was enhanced relative to the natural equilibrium living value).
There is one exception in which dating of single modern-period (i.e. within the nuclear era) bone samples can produce high precision estimations of year of birth. This is where the skeletal remains are of new-born or close to new-born babies. The shape of the ^{14}C bomb peak has been well constrained through extensive measurements of ^{14}C activities (Levin *et al.* 1994; Levin and Kromer 1997; Manning and Melhuish 1994; McGee *et al.* 2004) and the rapid annual changes provide the potential for a chronologically precise methodology (This also applies to components of human remains that exhibit either very fast carbon turnover). The bone collagen in infants is formed from the mother's dietary intake, and here, the ^{14}C will be relatively close to equilibrium with atmospheric levels. Broecker *et al.* (1959) derived an average value of <1 year for the period between initial fixation of carbon by plants and human consumption and a maximum lag of <6 months between carbon consumption and appearance in the blood. Therefore, a radiocarbon measurement made on the bone collagen should represent the ^{14}C activity of the atmosphere 1-2 years earlier than the year of death. The samples we analysed were all from children of <1 year of age and therefore a delay of 1-2 years should apply to them.

Under equilibrium conditions where the rate of production ≈ rate of decay, every living organism in the terrestrial biosphere is labelled with the same ^{14}C activity. On death, no more ^{14}C uptake occurs and only the decay process operates (see Figure 2).

$$^{14}_{6}C \longrightarrow {}^{14}_{7}N + \beta$$

This follows First Order Kinetics. For ^{14}C dating, re-arranging the first order decay equation ($A_t = A_0 e^{-\lambda t}$) for t gives:

$$t = \frac{1}{\lambda} \ln \frac{A_0}{A_t}$$

Where t = time elapsed since death, in years B.P. (Before Present, where present is the year 1950)

A_0 = equilibrium living activity
A_t = activity remaining after time t
λ = decay constant = ln2/5568 = 0.693/5568

A_0 cannot be measured directly as this is the equilibrium living activity. The A_0 activity is related to that of a reference standard whose activity is measured in the lab. A_t is the activity of the sample material now and is also measured in the lab. The primary standard used in radiocarbon dating is wood growing in the year 1890, which is pre-Suess and pre-nuclear weapons testing effects. The ^{14}C activity of this material was 13.56 dpm/gram of carbon (226 Bq kg^{-1} of carbon). This was measured in the mid-20th century and corrected for 60 years decay to the year 1950. This material was very limited and now a secondary standard is used. This is currently oxalic acid (termed Oxalic acid II or SRM 4990C) produced by the National Institute of Standards and Technology (Maryland, USA). This oxalic acid was synthesised from beet molasses in 1977 and 0.7459 x oxalic acid activity = 1890 wood activity = A_0 when both the wood and the oxalic acid are corrected for fractionation. SRM 4990C is commonly referred to as the primary standard.

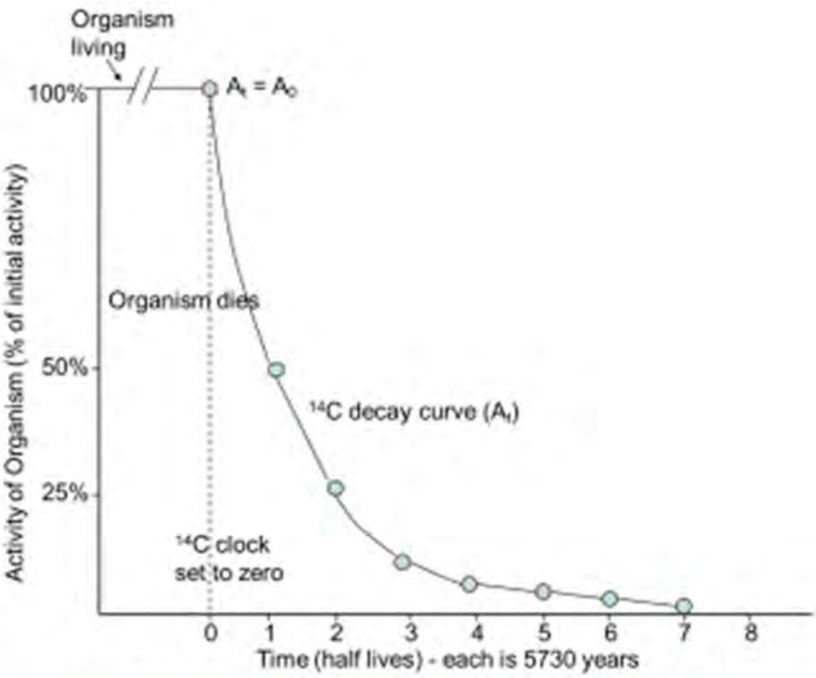


Figure 2: The decrease in ^{14}C activity of a sample organism with time.

Assumptions in the Method

There are 4 main assumptions in the radiocarbon method as follows:

1. The rate of production in the upper atmosphere has been constant throughout time.

2. The ^{14}C activity of the atmosphere and hence the biosphere, with which it is in equilibrium, has remained constant throughout time.

3. The rate of ^{14}C transfer between different reservoirs of the carbon cycle is rapid with respect to the average lifetime of ^{14}C.

4. The half-life is accurately known.

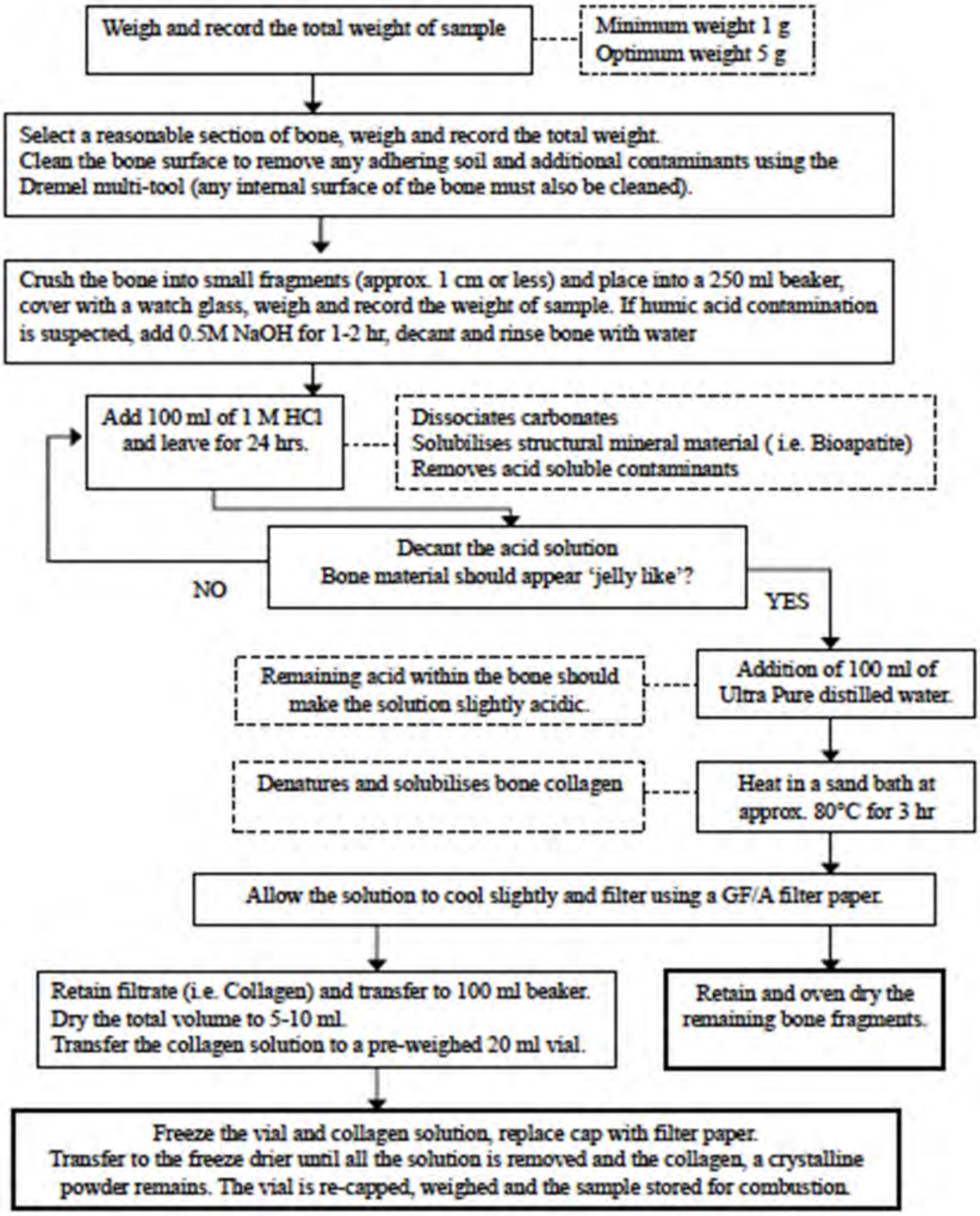
None are strictly correct!

For 1: Long term (millennia scale) and short term (century scale) fluctuations have occurred as discussed above.
For 2: The above variations in the rate of production will influence the ^{14}C activities of the atmosphere and biosphere. In addition, there can be changes in reservoir size, *e.g.* due to temperature changes causing increases and decreases in polar icecap cover.
For 3: The oceans are depleted relative to the atmosphere and hence organisms living in the oceanic environment will be depleted. They have a "reservoir age".
For 4: The original Libby half-life is still used to calculate ^{14}C ages, even although we know it to be incorrect.
For 1, 2 and 4: Dendrochronological curves and U/Th dating on coral samples/varve sequences solve many of the problems. The dendrochronological curves are derived by radiocarbon dating 10 year spans of tree rings from absolutely dated tree ring sequences, which are continuous from present day to approx. 12,600 years BP (before present where present is 1950AD). Absolute age is plotted against radiocarbon age to produce a calibration curve against which radiocarbon ages of samples can be calibrated on a calendar year time-scale. Beyond approx. 12,600 BP the calibration data are based on independent U/Th age measurements made on coral and varve sequences, etc.
For 3: This reservoir effect has been measured in many locations. For the UK, the apparent age on death appears to be around the global average of 400 years but is variable through time (eg. Ascough *et al.* 2004).

SAMPLE PREPARATION

Bone consists of two basic fractions. The inorganic fraction is primarily calcium phosphate with an apatite-like structure, but incorporating a small percentage of carbonate (0.5-1% by weight) as a substitute for phosphate in the crystal lattice. The organic fraction is primarily a protein termed collagen.
Where the bone has not been cremated, our preferred procedure is to extract the collagen as a partially hydrolysed fraction (gelatin), followed by freeze drying.
Sub-samples were removed from each of the 6 bones, cleaned thoroughly and subjected to the collagen preparation process illustrated in the following flow diagram.

Preparation of bone collagen



Conversion of collagen to graphite for accelerator mass spectrometry (AMS) radiocarbon measurement

Combustion of the collagen samples for radiocarbon dating was undertaken according to the method of Vandeputte *et al.* (1996). Approx. 14-16 mg sub-samples of collagen were weighed into quartz combustion tubes containing copper oxide as a source of oxygen and silver foil to mop up halides and other contaminants. The combustion tubes were then evacuated, sealed and placed in a furnace at 850°C overnight. The CO_2 produced during the combustion was cryogenically purified and 3 ml sub-samples were converted to graphite for subsequent AMS measurement using the method of Slota *et al.* (1987).

SAMPLE MEASUREMENT

Radiocarbon (^{14}C) Measurements

^{14}C measurements on the graphite preparations was undertaken using our 250 kV Single Stage Accelerator Mass Spectrometer (SSAMS), manufactured by National Electrostatics Corporation. This spectrometer features a high intensity sputter ion source with a 134 sample capacity.

The SUERC Radiocarbon Laboratory does not have certification under the BS5750/ISO9000 Quality Assurance schemes, however, the laboratory takes part in all the major international inter-calibration studies and has been at the forefront in organising five of the last six. In addition, we have a fully implemented Quality Assurance manual which details all of the procedures employed in the laboratory and demonstrates how each sample is tracked through the laboratory. Details recorded include pre-treated sample yields, sample carbon graphitisation yields, etc.

The laboratory uses the primary ^{14}C standard, SRM-4990C, for all estimates of modern reference standard activity. Wheels of up to 134 samples, including standards, are measured and since measurements of such large numbers of samples can last several days, our procedures have to cope with changes in measurement conditions. To this end, samples are measured to completion in groups of 10 in only a few hours, with Oxalic acid II primary standards spanning groups for intergroup consistency. Each group of 10 samples contains: (i) one Oxalic acid II primary standard, (ii) one humic acid secondary standard of less than 1 half-life in age (used in 2 international inter-calibration studies: C-14 Cross-check Peat Sample and VIRI Sample T; the consensus value from the former study is 3374 ± 9 y BP and from VIRI it is 3360 ± 3 y BP), (iii) either a modern secondary standard material (TIRI Sample A (barley mash); the consensus value from this study is $F^{14}C = 1.1635 \pm 0.0041$ (when the activity is higher than the modern value it is expressed as a fraction modern ($F^{14}C$) rather than a radiocarbon age), or a background standard (interglacial wood, infinite age bone or geological carbonate depending on the type of unknowns being measured), and (iv) 7 unknowns. Such rapid analysis is relatively insensitive to longer-term drifts and changes are quickly apparent in the fast repeat measurements of individual samples, including primary and secondary standards. Operator intervention, to adjust the spectrometer or to change sample measurement parameters, can be immediate; each sample is automatically repeatedly measured in intragroup rotation until the sample total counting statistics and the scatter of the repeat $^{14}C/^{13}C$ measurements exceeds a quality threshold of typically 3‰, disregarding early inconsistent measurements as necessary.

Finally, time trends remaining in the completed data sets can be compensated for in subsequent data reduction and normalization.

Stable Isotope Measurements

Further 0.6 mg samples (approx.) of collagen were weighed into tin capsules for stable isotope measurements (^{13}C and ^{15}N and C/N ratio) using a continuous-flow isotope ratio mass spectrometer (Thermo Scientific Delta V Advantage (Bremen, Germany) coupled to a Costech ECS 4010 elemental analyser (EA) (Milan, Italy) fitted with a pneumatic autosampler. The EA is coupled to the mass spectrometer via a ConfloIV™ and samples are combusted in a single reactor containing tungstic oxide and copper wires at 1020°C to produce N_2 and CO_2. The gases are then separated in a 2 m stainless steel Porapak QS 50-80 mesh GC column heated to 70°C. Helium (100 ml/min) is used as a carrier gas throughout the procedure. N_2 and CO_2 enter the mass spectrometer via an open split arrangement within the ConfloIV™ and are analysed against their corresponding reference gases.
For every ten unknown samples, in-house gelatine standards, which are calibrated to the international reference materials USGS40, USGS41, IAEA-CH-6, USGS25, IAEA-N-1 and IAEA-N-2, are run in duplicate. Results are reported as per mil (‰) relative to the internationally accepted standards VPDB and AIR with 1σ precisions of ± 0.2‰ and ± 0.3‰ for $\delta^{13}C$ and $\delta^{15}N$, respectively. Any results for bone samples that have molar C/N ratios outside the range of 2.9-3.6 would be discarded as they would be deemed to represent collagen that has undergone post-depositional alteration (DeNiro, 1985).

RESULTS

We analysed the ^{14}C, $\delta^{13}C$ and $\delta^{15}N$, and determined the C/N ratio in the samples of collagen that were isolated from our samples referenced GU-42246 to GU-42251. The results are presented in Table 2 and the quality assurance results for the batch of analyses that included GU-42246 to GU-42251 are shown in Table 1.

QA Sample	Sample type	Consensus Age (years BP) or Fraction Modern ($F^{14}C$) ± 1σ	Age (years BP) or Fraction Modern ($F^{14}C$) ± 1σ (this batch)
C-14 Crosscheck/ VIRI Sample T	Humic acid	3374 ± 9 y BP 3360 ± 3 y BP	3349 ± 29 y BP
TIRI Sample A	Barley Mash	1.1635 ± 0.0041	1.1659 ± 0.0018

Table 1: Radiocarbon QA results for the batch of samples containing samples GU-42246 to GU-42251.

The QA data demonstrate that results in this batch of analyses are accurate as both the mean Humic Acid and Barley Mash secondary standard values are well within error of the consensus values produced by the worldwide radiocarbon community. The data are also precise as the standard deviation on the Humic Acid values is 29 years while the standard deviation on the fraction modern values for the Barley Mash standards is 0.0018.

Analysis Code	Exhibit Ref.	Bone Id.	$\delta^{13}C$ (‰)	$\delta^{15}N$ (‰)	C/N Ratio	Fraction modern ± 1σ
SUERC-69881	LL001	Left Femur	-19.2	+9.7	3.4	0.9851 ± 0.0033
SUERC-69882	LL002	Left Temporal	-19.7	+10.1	3.5	0.9734 ± 0.0035
SUERC-69883	LL003	Right Parietal	-19.6	+9.9	3.5	0.9754 ± 0.0035
SUERC-69884	LL004	Left Temporal	-21.2	+9.5	3.5	0.9746 ± 0.0035
SUERC-69885	LL005	Right Parietal	-21.9	+9.6	3.6	1.0639 ± 0.0038
SUERC-69886	LL006	Left Ulna	-21.5	+9.7	3.6	1.0641 ± 0.0039

Table 2. Radiocarbon and stable isotope results for bone samples GU-42246 to GU-42251 (Our Analysis codes: SUERC-69881 to SUERC-69886).

The C/N ratios for the samples of isolated collagen are within the limits for collagen that is unaltered (accepted range is 2.9-3.6) and therefore are deemed suitable for radiocarbon and stable isotope measurements.

DISCUSSION

The stable isotope values for the 6 samples are fairly typical of diets that are very dominantly derived from terrestrial resources. Therefore, there is no requirement to make any allowance for a marine reservoir effect. The calibration of the samples (LL001-LL004) with fraction modern values of <1 to produce calendar age ranges were undertaken using OxCal version 4.2 (IntCal 13 curve), while those with fraction modern values >1 were calibrated using the Post-bomb atmospheric Northern Hemisphere Zone 1 Curve (Bronk Ramsey 2013). The calibrations are illustrated in Figures 3-8. For some of the calibrations where the $F^{14}C$ values were in the 0.97-0.98 range, the later ranges do not have end-points, however, these cannot be beyond 1955 as at this point the $F^{14}C$ value in the atmosphere exceeds 1. I would not pay too much attention to the probabilities as these tend to reflect the shape of the curve, which is very complex from 1650 AD onwards, rather than true probabilities for the ages.

Similarly, for LL005 and LL006 which calibrate within the nuclear era, the later age ranges again do not have end-points. I checked these against the Queen's University Belfast calibration programme (CaliBOMB) and got values of 2009 for both. Again, do not pay too much attention to the probabilities. The small probabilities for the earlier age ranges (1956-1957) are due to the fact that the curve is very steep at this point while for the later age ranges it is quite a shallow curve. The calibrated age ranges are illustrated in Table 3.

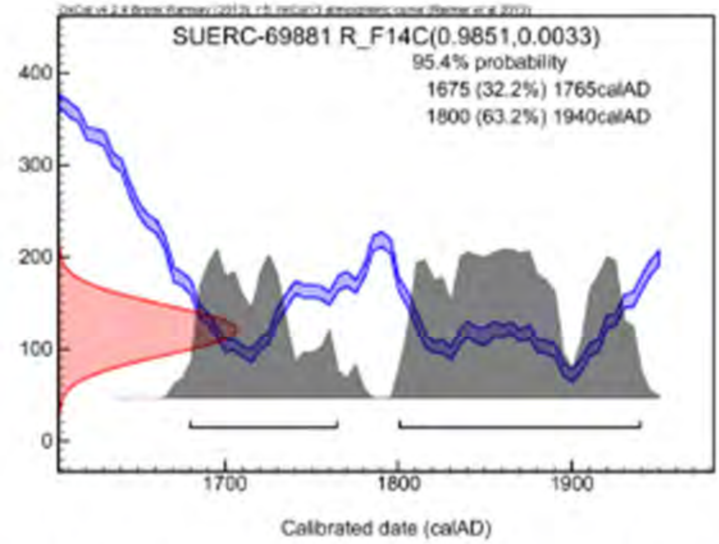


Figure 3: Calibration of bone sample GU-42246 (LL001) (Our analysis code SUERC-69881).

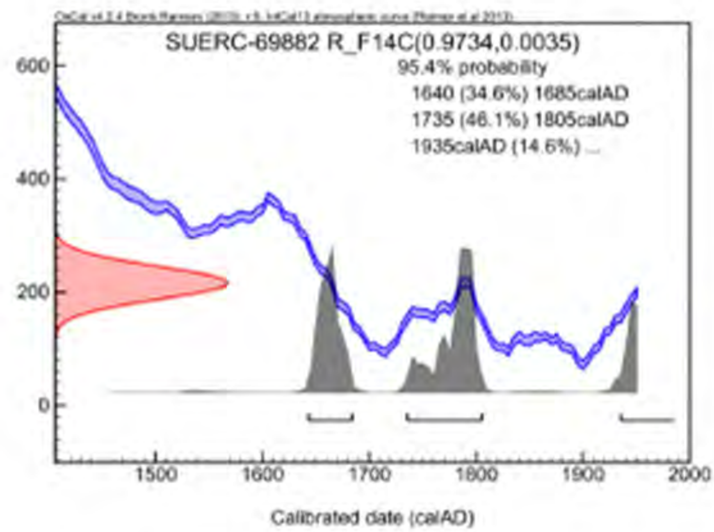


Figure 4: Calibration of bone sample GU-42247 (LL002) (Our analysis code SUERC-69882).

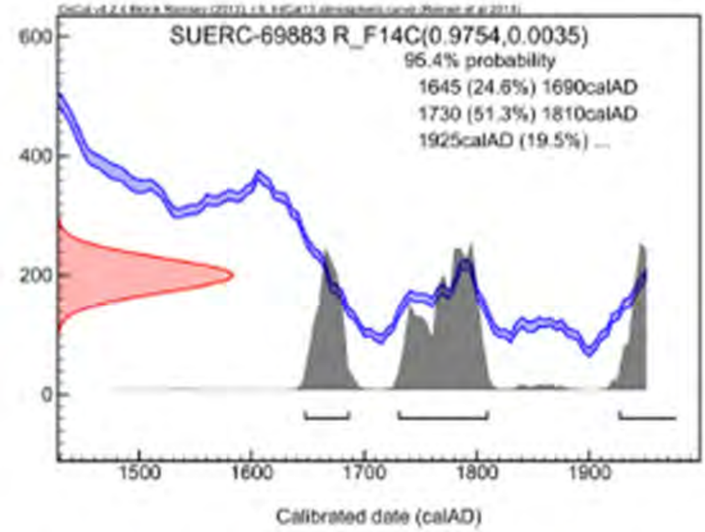


Figure 5: Calibration of bone sample GU-42248 (LL003) (Our analysis code SUERC-69883).

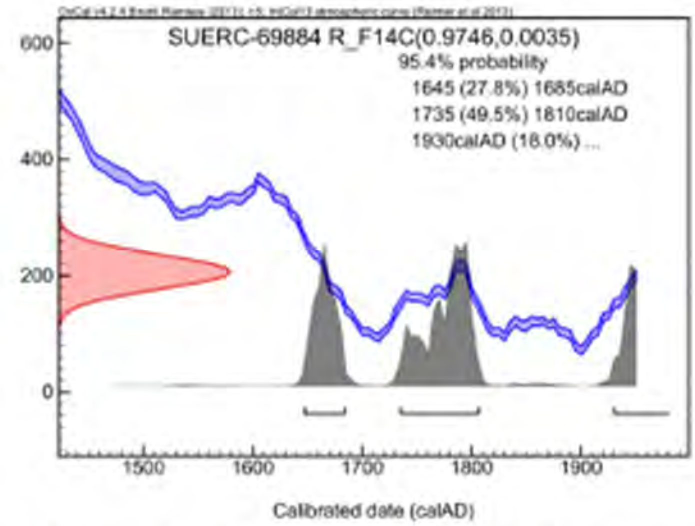


Figure 6: Calibration of bone sample GU-42249 (LL004) (Our analysis code SUERC-69884).

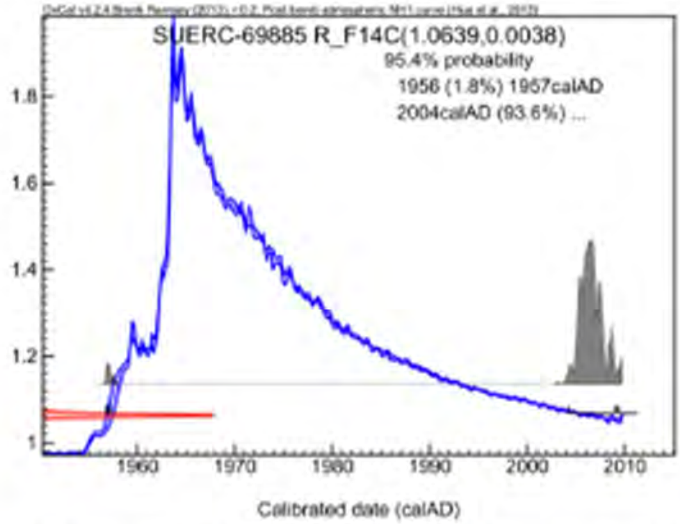


Figure 7: Calibration of bone sample GU-42250 (LL005) (Our analysis code SUERC-69885).

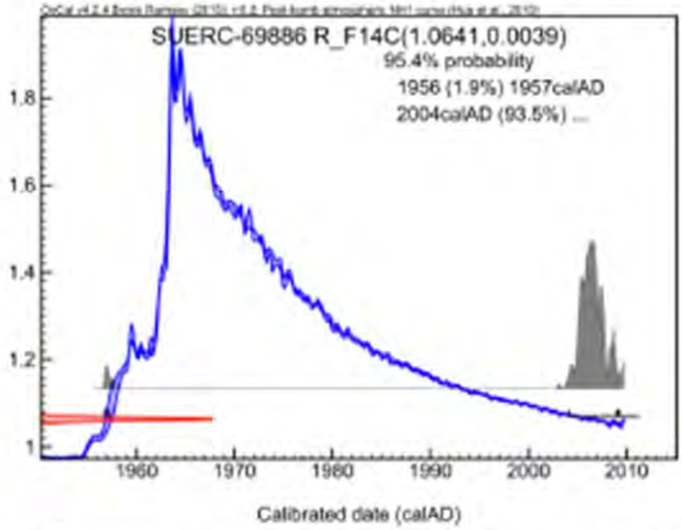


Figure 8: Calibration of bone sample GU-42251 (LL006) (Our analysis code SUERC-69886).

Sample	Calibrated Age Ranges (years AD)	Calibrated Range of Interest
LL001	1675-1765; 1800-1940	1800-1940
LL002	1640-1685; 1735-1805; 1935-1955	1935-1955
LL003	1645-1690; 1730-1810; 1925-1955	1925-1955
LL004	1645-1685; 1735-1810; 1930-1955	1930-1955
LL005	1956-1957; 2004-2009	1956-1957
LL006	1956-1957; 2004-2009	1956-1957

Table 3. Calibrated age ranges for LL001-LL006

CONCLUSIONS

The measured fraction modern values for LL001 to LL004 are all significantly <1 and all have multiple, possible calibrated age ranges, which is fairly typical for fraction modern ($F^{14}C$) values around 0.97-0.98. These typically produce calendar ages in the pre-modern 1650-1950 AD range as defined by Taylor *et al.* (1989). However, it is important to note that they all produce age ranges within the period when the Home operated. LL005 and LL006 have $F^{14}C$ values significantly greater than 1 and this clearly puts the years of death within the nuclear era (in fact, post-1955). Again, the earlier range of 1956-1957 is within the period of operation of the Home. If I apply a lag of 1-2 years as described by Broecker *et al.* (1959), this would put their years of death around 1956-1959.

REFERENCES

Arneborg, J., Heinemeier, J., Lynnerup, N., Nielsen, H.L., Rud, N., Sveinbjornsdottir, A.E. 1999. Change of diet of the Greenland Vikings determined from stable isotope analysis and ^{14}C dating of their bones. *Radiocarbon* **41**, 157-168.

Ascough, P.L., Cook, G.T., Dugmore, A.J., Barber, J., Higney, E., and Scott, E.M. (2004) Holocene variations in the Scottish marine radiocarbon reservoir effect. *Radiocarbon* **46**, 611-620.

Broecker WS, Schulert A, Olson EA (1959) Bomb Carbon-14 in human beings. *Science* **130**, 331–332.

Bronk Ramsey, C. (2013) OxCal V 4.2.4.

Damon, P.E., Cheng, S. and Linick, T.W. (1989) Fine and hyperfine structure in the spectrum of secular variations of atmospheric ^{14}C. *Radiocarbon* **31**, 704-718.

DeNiro, M.J. (1985) Postmortem preservation and alteration of in *vivo* bone collagen isotope ratios in relation to palaeodietary reconstruction. *Nature* **317**, 806-809.

Elsasser, W., Ney, E.P. and Winckler, J.R. (1956) Cosmic-ray intensity and geomagnetism. *Nature* **178**, 1226-1227.

Hedges, R.E.M., Clement, J.G., Thomas, C.D.L. and O'Connell, T.C. (2007) Collagen turnover in the adult femoral mid-shaft: Modeled from anthropogenic radiocarbon tracer measurements. *American Journal of Physical Anthropology* **133**, 808-816.

Hua, Q., Barbetti, M., and Rakowski, A. J. (2013). Atmospheric Radiocarbon for the Period 1950-2010. ***Radiocarbon*** **55**(4), 2059-2072.

Levin, I., Kromer, B., Schoch-Fischer, H., Bruns, M., Münnich, M., Berdau, D., Vogel, J.C., Münnich, K.O. (1994) $\delta^{14}CO_2$ record from Vermunt. In Trends: A Compendium of Data on Global Change. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tenn., U.S.A.

Levin, I., Kromer, B. (1997) Twenty years of atmospheric CO_2 observations at Schauinsland. *Radiocarbon* **39**, 205–218.

Manning, M.R., Melhuish, W.H. (1994) Atmospheric ^{14}C record from Wellington. In Trends: A Compendium of Data on Global Change. Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, U.S. Department of Energy, Oak Ridge, Tenn., U.S.A.

McGee, E.J., Gallagher, D., Mitchell, P.I., Baillie, M., Brown, D., Keogh, S.M. (2004) Recent chronologies for tree rings and terrestrial archives using ^{14}C bomb fallout history. *Geochim Cosmochim Acta* **68**, 2509–2516.

Russell, N., Cook, G.T., Ascough, P.L. and Scott, E.M. (2015) A period of calm in Scottish seas: A comprehensive study of ΔR values for the northern British Isles coast and the consequent implications for archaeology and oceanography. *Quaternary Geochronology* **30**, 34-41.

Slota, P.J., Jull, A.J.T., Linick, T.W., Toolin, L.J. (1987) Preparation of small samples for ^{14}C accelerator targets by catalytic reduction of CO. *Radiocarbon* **29(2)**, 303-6.

Sternberg, R.S. (1992) Radiocarbon fluctuations and the geomagnetic field. In *Radiocarbon After Four Decades*, R.E. Taylor, A. Long and R.S. Kra, eds, Springer-Verlag, pp 93-116.

Stuiver, M. (1961) Variations in radiocarbon concentration and sunspot activity. *Journal of Geophysical Research* **66**, 273.

Suess, H.E. (1953) Natural radiocarbon and the rate of exchange of carbon dioxide between the atmosphere and the sea. In *Nuclear Processes in Geologic Settings*, W. Aldrich, ed., University of Chicago Press, Chicago, pp 52-56.

Suess, H.E. (1955) Radiocarbon concentration in modern wood. *Science* **122**, 415–417.

Taylor, R.E., Suchey, J.M., Payen, L.A., Slota, P.J. Jr (1989) The use of radiocarbon (^{14}C) to identify human skeletal materials of forensic science interest. *Journal of Forensic Science* **34**, 1196–1205.

Vandeputte, K., Moens, L. and Dams, R. (1996). Improved sealed-tube combustion of organic samples to CO_2 for stable isotope analysis, radiocarbon dating and percent carbon determinations. *Analytical Letters* **29**, 2761–73.

Addendum to Radio Carbon Dating Report of Professor Gordon T Cook

The measured fraction modern values for LL001 to LL004 are all significantly <1 and all have multiple, possible calibrated age ranges, which is fairly typical for fraction modern ($F^{14}C$) values around 0.97-0.98. These typically produce calendar ages in the pre-modern 1650-1950 AD range as defined by Taylor et al. (1989). The probabilities all reflect the area under the blue curve and so, where the curve is very steep, the probability is low. Therefore, I would disregard these as being unlikely to reflect the true probability of when death occurred but it is important to note that they all produce age ranges within the period when the Home operated. LL005 and LL006 have $F^{14}C$ values significantly greater than 1 and this clearly puts the years of death within the nuclear era (in fact, post-1955). Again, the earlier range of 1956-1957 is at a point when the blue curve is rising very steeply and hence the area under the curve (and consequently the probability) will be low. Again, I would discount the low probability for this age range as being an accurate reflection of when death occurred. This range of 1956-1957 is also within the period of operation of the Home and if I apply a lag of 1-2 years, as described by Broecker et al. (1959), this would put their years of death around 1956-1959.

Signed: Gordon T Cook

Gordon T Cook

Appendix IX: Environmental Sampling Report

James Hutton Limited

CRIMINAL Expert Certificate CIVIL Expert Certificate

Report

For Niamh McCullagh
The Mother and Baby Homes Commission of Investigation

(Criminal Procedure Rules [2015] Parts 16 and 19; Criminal Justice Act 1967, s. 9)

Report of Professor Lorna DAWSON and Dr Bob MAYES

Qualifications BSc, PhD, C.Sci, F.I.Soil Sci, FRSA (LD); BSc, MSc, PhD (BM),

Age Over 18

Occupation Soil Scientist and Organic Marker Chemist

Address James Hutton Institute
Craigiebuckler
Aberdeen
AB15 8QH

This report, consisting of 25 pages, is true to the best of our knowledge and belief and we make it knowing that, if it is tendered in evidence, we shall be liable to prosecution if we have wilfully stated in it anything which we know to be false or do not believe to be true.

We understand our duty as expert witnesses to the court to provide independent assistance by way of objective unbiased opinion in relation to matters within our expertise. We will inform all parties and where appropriate the court in the event that our opinion changes on any material issues.

We further understand that our duty to the court overrides any obligation to the party from whom we received instructions.

The examinations we make depend to some extent on items submitted to us and on information provided regarding the alleged circumstances of the case. Our conclusions normally relate to our examinations, those of our colleagues specified in this report, and of those submitted items and to the significance of our findings in the light of the alleged circumstances of the case. We are prepared to make any further examinations as requested by the Prosecution or the Defence, and we are prepared to test any alternative scenarios which may be put to us. If any information we have used should change significantly, or if further examinations are required, then we may need to revise our conclusions.

Signed Lorna Dawson Dated the 6th Dec 2016.

Signed R.N. Mayes Dated the 6th Dec 2016

Table of Contents

1. Qualifications and Experience

Prof. Lorna DAWSON

I am employed as a principal research scientist at the James Hutton Institute, Aberdeen, Scotland, where I am Head of the Soil Forensics Section and hold the qualifications of BSc (Honours) Geography (Edinburgh University, 1979), and a PhD in Soil Science (Aberdeen University, 1984). I am a visiting Professor in Forensic Science at the Robert Gordon University. I am a Fellow of the British Society of Soil Science, a Fellow of the Royal Society of the Arts, a Chartered Scientist and hold an Expert Witness certificate in both Criminal and Civil Law (Cardiff University, 2011, 2012). I have published widely on the subject of forensic soil science; published over 80 refereed publications, books and book chapters. I am an Expert Advisor with the National Crime Agency, have worked with numerous police forces in Scotland, England, Wales, Ireland & Australia over the last 12 years and have advised on over 80 cases, written over 70 Expert Witness reports, and presented evidence in 9, in the UK and overseas. During the past 12 years I have encountered the evidence type involved in this case on several occasions.

Dr Bob MAYES

I am a Research Associate at the James Hutton Institute where I was previously head of the Ecological Sciences GC and GC-MS laboratories, and hold the qualifications PhD from Queen's University of Belfast, MSc in Animal Nutrition from the University of Aberdeen and BSc in Physiology and Biochemistry of Farm Animals from Reading University. I am an expert in the analysis of wax markers and my research interests revolve around the application of this biomarker technology to measuring dietary intake, digestibility and plant species composition in grazing herbivores and to the characterisation of soil organic matter as applied in criminal investigations. I have worked with a number of police forces in Scotland, England, Wales & Ireland over the last 6 years, have written over 16 Expert Witness reports, and presented evidence in court with two of them. During the past 6 years I have encountered the evidence type involved in this case on a number of occasions.

2. Summary of findings

The sample examined is not a typical soil. It was shown from GC-MS analysis that there are markers of faeces (cholesterol, faecal stanols and faecal bile acids) in the sample. The observed patterns of these individual markers were typical of human faeces, and not of faeces from any herbivore (e.g. sheep, cattle, horses or rabbits), pigs or dogs. However, despite the high organic matter content of the sample, the concentrations of faecal markers were extremely low, compared with levels expected from decomposed faecal material (such as sewage sludge, septic tank sludge or manure). Thus either the faecal material had been considerably diluted by the presence of non-faecal organic matter, or the faecal markers had come from another source. The possibility that the faecal markers had originated from decomposing cadavers cannot be ruled out. The fatty acid, 10-hydroxy stearic acid, which is a recognised body decomposition marker, was found in the sample at low levels, but its origin in this case was not clear, because it is also found in human faeces. Any association of cadaver decomposition with the presence of faecal bile acids has yet to be established.

An unusual feature about the *n*-alkane/alcohol/sterol results of the sample examined was the exceptionally high levels of the plant sterols, β-sitosterol and campesterol, together with low (but detectable) concentrations of plant-wax *n*-alkanes and fatty alcohols. The observed *n*-alkane and long-chain fatty alcohol patterns were typical of those found in grasses and other higher plants, but their low concentrations relative to the plant sterol levels in the sample suggest that decomposed plant material was unlikely to be the source. We have also found unusually high levels of plant sterols in some samples of pig faeces, but in that particular case the pig feed (which we had analysed) was rich in β-sitosterol and campesterol.

There is the possibility that it was infant matter that was in the sample (including infant faecal matter) and that the high levels of plant sterols we detected in the sample could be as a result of infants being fed with formula milk containing vegetable oils. (Nearly all formula milks contain vegetable oils). The relative levels of plant sterols, *n*-alkanes and fatty alcohols in vegetable oils are similar to those found in the current analysed sample. Furthermore, although the patterns of *n*-alkanes and fatty alcohols can vary according to the type of vegetable oil, the patterns found in the sample examined were compatible with certain individual oils, or mixtures of oils.

The concentration patterns of stanols and sterols and hydrocarbons found in the sample are not compatible with that of sewage from human adults or from individuals eating solid food.

The alcohol/sterol fraction and hydrocarbon fraction profiles suggest that the sample examined is not material originating from a sewage treatment plant, septic tank or cesspit. It is unlikely that the specific location of the questioned case sample was a receptacle for sewage.

The sample does contain indicators which suggest that human faeces are present. However, the markers present are not compatible with that of sewage from human adults or children eating solid food. It has not originated wholly from a sewage treatment plant or wholly from adult faeces.

3. Information/Circumstances of Case

I, Lorna DAWSON, received an email from Forensic Archaeologist Niamh McCULLAGH, agent for The Mother and Baby Homes Commission of Investigation, on 25th October 2016, to enquire if we could examine a soil sample to establish whether there was human faecal matter contained within it.

4. Items Received

A sample labelled MBHCOI_TM1016, Exhib No. LLO16 Tr 1A, Feature 1B, Earth from Bone LL005, 6 and 7 was received into the James Hutton Institute Forensic Laboratory, lab 234, Aberdeen, on 4th November 2016.

5. Request or Purpose of Examination

We were requested that we, in the Soil Forensic Unit, examine and analyse the sample for human faecal material to establish if a system built for human effluent, from which the sample was taken, was ever used for this purpose.

6. Assumptions

It is assumed the sample was collected in a rigorous manner and that the sampling was carried out with due care and by adhering to established forensic sampling protocols.

7. Use of Assistants

In undertaking the work in this case I was assisted by other members of the Soil Forensic Unit Laboratory staff. Their involvement is described in the forensic case files and I have taken their contributions into account when we prepared this report. The involvement of other staff is fully recorded in case notes available for inspection at the laboratory if necessary. Mrs Jasmine ROSS, forensic laboratory manager, assisted myself in examining the sample, captured photographs, analysed the samples for organic markers and prepared the audit trail (Appendix 2, Table 1). Dr Bob MAYES interpreted the chromatograms for faecal markers. Dr Andy MIDWOOD, Head of Environmental and Biochemical Sciences Group and Prof. Colin CAMPBELL, CEO, James Hutton Institute, reviewed this statement. Dr Barry THORNTON analysed the sample for isotopic C and N. Prof Steve HILLIER excluded the crystals as not being asbestos by visual examination.

8. Nature of Examination

Soil is a mixture of both inorganic and organic material (Dawson and Hillier, 2010: Dawson and Mayes, 2014). The inorganic material can be characterised by its elemental composition (see glossary, Appendix 3) which generally reflects the geological material from which it was derived. The organic material reflects the plant and animal material having been deposited or decomposed within that soil and also human organic inputs to the soil (Dawson and Mayes, 2014). A combination of gas chromatography (GC) and gas chromatography-mass spectrometry (GCMS) can be used to characterise and identify many organic compounds in soils.

This report describes the soil examination and the organic analysis of the sample received on the 4th November 2016.

A full record of the work done in this case is available for inspection at Laboratory 234, the James Hutton Institute, Aberdeen.

An audit trail is in Appendix 1. A list of references used is in Appendix 2. A glossary of technical terms is in Appendix 3.

9. Results

Soil description

The soil samples were examined under a macro lens and then under a microscope at times 20 magnification.

Table 2. Description of soil samples examined

Exhibit/Item Number	Location	Mineral Composition	Organic material and other fragments	Colour (Munsell colour chart)
Exhib No. LLO16 Tr 1A, Feature 1B	Earth from Bone LL005, 6 and 7	Few white stones rounded and sub-rounded, and angular and sub-angular. (calcite?), white aggregates, gravel, anthracite, red brick.	Woody bark, blue fibre, small bone fragments, green grass blades, dead deciduous leaf material, glass, paint. Possible asbestos fibres? (white/clear/needle like clusters of crystals, originally thought to be asbestos").	2.5Y 3/1 (very dark grey).

The soil samples were sieved through a 1mm sieve to provide two fractions. The finer fraction was prepared for subsequent organic profile characterisation. The coarser fraction was retained (Appendix 1, Table 1, Audit trail). Images of the finer fraction are in Appendix 5.

Visually the sample appeared similar, when compared with images of previous samples examined, to a "black earth" sample from (Barbara von der LUHE, 21 Jan 2013), which was known to have originated from material adjacent to a human cadaver. Small bone like fragments were observed in the sample (visual only; unconfirmed by anthropologist). White crystals were confirmed through visual assessment by mineralogist to not be asbestos. There were some grass leaf material in the sample; it is unclear whether those may have fallen into the sample on collection. These were not included in the sample analyzed.

Soil Organic Marker Analysis

Hydrocarbons

Figure 1 shows the hydrocarbons extracted from the case sample analysed by GC (fitted with a flame ionisation detector).

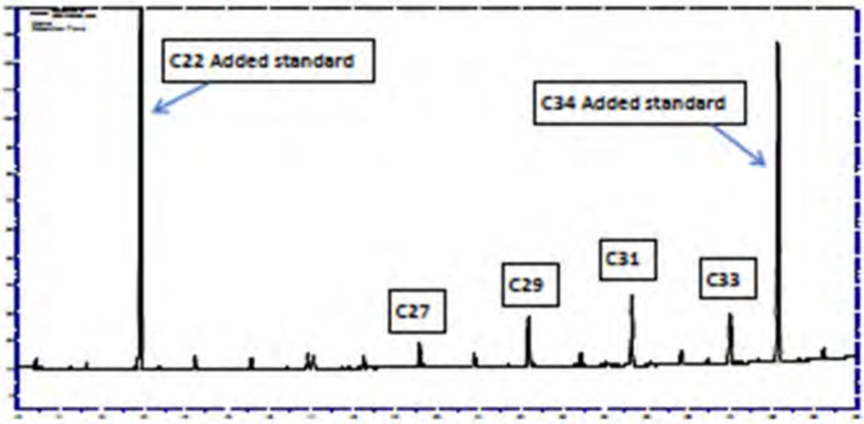


Figure 1. Gas chromatogram of the hydrocarbon fraction obtained from the analysed case sample.

The hydrocarbons found in the sample were odd-chain *n*-alkanes, dominated by hentriacontane (C31), nonacosane (C29), tritriacontane (C33) and heptacosane (C27). Shorter odd-chain *n*-alkanes and even-chain *n*-alkanes were also present at much lower levels. The *n*-alkane and alcohol patterns were typical of the patterns found in grasses and a large number of other higher plants but the concentrations were low (e.g. the C31 *n*-alkane was 23mg/kg in the sample examined, whereas in a typical grassland concentrations would range between 100 and 400 mg/kg).

Fatty alcohols, sterols and stanols

The fatty alcohol/sterol fractions extracted from the sample were analysed by GCMS and the results are shown in Figures 2 and 3. Figure 2 shows the complete chromatogram (total ion count) in which the even-chain fatty alcohols have been are identified. Figure 3 represents a partial chromatogram of the same analysis, showing the sterols and stanols present.

Even-chain fatty alcohols were detected, with 1-hexacosanol (C26), 1-tetracosanol (C24) and 1-octacosanol (C28) dominating. Also present were 1-eicosanol (C20) and 1- triacontanol (C30). 1-Docosanol (C22) was also detected, but co-eluted with a much larger amount of dioctyl phthalate, which can be leached out of various plastics (it cannot be ascertained if this substance was present in the case sample itself, or appeared as a contaminant from plastic sample packaging material).

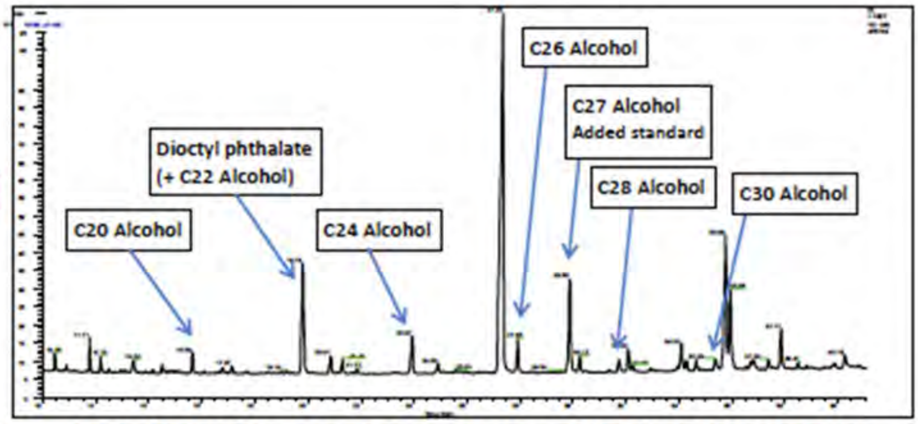


Figure 2. GC-MS (total ion count) chromatogram of the alcohol/sterol fraction obtained from the analysed case sample. Fatty alcohol peaks are labelled.

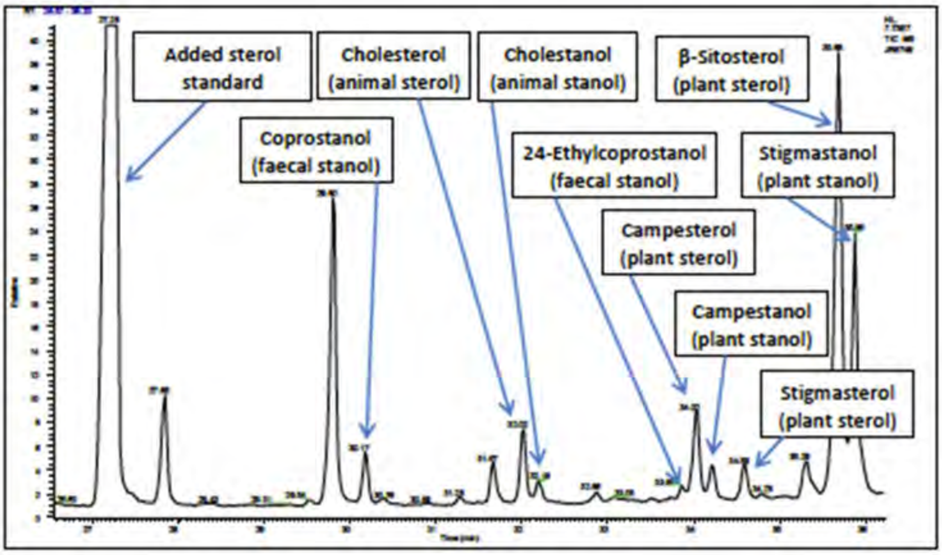


Figure 3. Partial GCMS (total ion count) chromatogram of the alcohol/sterol fraction obtained from the analysed case sample. Sterol and stanol peaks are labelled.

The pattern of fatty alcohols present was typical of the patterns found in grasses and a large number of other higher plants. The concentrations were much lower than in any grassland topsoils previously examined.

The case sample contained β-sitosterol, campesterol and stigmasterol, which are plant sterols found in most surface soils. Also present was the animal sterol, cholesterol, which is also very common in soils. The plant stanols, stigmastanol and campestanol, which are commonly found in soils as a result of microbial transformation of the plant sterols, were found in the case sample. Cholestanol was also present; this was likely formed in the soil by microbial action on cholesterol. Coprostanol and 24-ethyl coprostanol were also detected. These are occasionally found in soil samples and originate from faecal material by respective hydrogenation of cholesterol and β-sitosterol in the gut of animals, including humans. Trace amounts of epicoprostanol and 24-ethyl epicoprostanol were detected (not shown, but data available upon request) by selecting relevant single-ion fragments to create derived GCMS chromatograms (Note that 24-ethyl epicoprostanol co-elutes with campesterol and could not be seen in the total ion count (TIC) chromatograms shown in Figures 2 and 3.). Whilst the concentrations of plant sterols and stanols in the sample were relatively high, the levels of faecal stanols in the sample were low. The concentrations were much lower than in any soils previously examined.

Faecal bile acids and 10-hydroxystearic acid

An acid fraction was obtained from the case sample and was treated such that carboxyl groups on the acid molecules were methylated, and any hydroxyl groups present were silylated (as trimethylsilyl ethers); this was to render hydroxyl-acid compounds analysable by GCMS (in TIC mode). Single-ion GCMS chromatograms were generated from the TIC chromatographic data, following relevant ions for the bile acids, lithocholic acid (m/z = 372), deoxycholic acid (m/z =255) and hyodeoxycholic acid (m/z = 355), and for 10-hydroxystearic acid (m/z =273). Examination of the derived GCMS chromatograms indicated that lithocholic acid, deoxycholic acid and 10-hydroxystearic acid were detected at very low levels in the case sample; hyodeoxycholic acid was absent. The relevant GCMS chromatograms are not shown in this report, but are available upon request.

Total carbon and nitrogen, and stable isotope (13C and 15N) content

After drying and milling the sample, the total organic carbon and nitrogen content and respective ^{13}C and ^{15}N isotopes were determined by continuous flow - isotope ratio mass spectrometry linked to an elemental analyser. The total organic C content of the sample was 40% w/w.

Table 3 Isotope values of the analysed sample

$\delta^{13}C$ (‰)	$\delta^{15}N$ (‰)
-24.40	11.6

Table 3 above shows that the isotope values for the sample were outliers compared to a large collection of top soil samples collected across Scotland and examined previously in a study by Thornton et al, 2015 (n=182). The mean (and standard deviation) isotopic values for the samples in the study by THORNTON were −27.7 ± 0.9‰ for ^{13}C and 3.6 ± 1.7‰ for ^{15}N. This corroborates the indications from microscopic examination that this sample was not a conventional 'soil'.

10. Interpretation and Conclusions

Replies to questions posed by Niamh McCULLAGH are listed below:

What is the sample?

Examination suggests that the sample is predominantly organic in nature. There are some traces of grass blades and woody material within the sample, tiny bone fragments (unconfirmed by anthropologist) within the sample, coal fragments, some brick, some crystals of unknown origin (confirmed as NOT being asbestos), few mineral grains and fibres of various colours. It does not appear to be a soil; there is very little natural soil aggregate formation, and only a few mineral grains intermixed. The sample contains some features of soil, although it was outside the normal isotopic N and C of over 100 soil samples previously examined across Scotland. It was not composed of predominantly plant organic material or of mineral material and most closely resembles a "black earth" sample we had previously examined which originated from close to a decomposing human body.

The main unusual feature about the alcohol/sterol results as determined was the exceptionally high levels of β-sitosterol and campesterol, relative to those of *n*-alkanes and fatty alcohols found in surface soils and vegetation. The plant sterols in the questioned sample were also much higher in concentration relative to faecal stanols and cholesterol in reference samples of faeces, sewage sludge, manures and materials associated with cadaver decomposition. We have also found unusually high levels of plant sterols in some samples of pig faeces, but in that particular case the pig feed (which we had analysed) was rich in β-sitosterol and campesterol.

The main compound which was of plant origin in the sample was the plant sterol β-sitosterol. There was also some campesterol, stigmasterol and stigmastanol and also *n*-alkanes and long-chain fatty alcohols of a typical plant pattern.

The high plant sterols which were detected in the sample could be from faeces from individuals fed on substances containing vegetable oils. The relative levels of plant sterols, *n*-alkanes and fatty alcohols in vegetable oils are similar to those found in the analysed sample (pers comm, Dr MAYES). Furthermore, although the patterns of *n*-alkanes and fatty alcohols can vary according to the type of vegetable oil, the patterns found in the sample were compatible with certain individual oils, or mixtures of oils.

Could there be human faeces in the sample?

The overall concentrations of faecal stanols were measurable, but were low. The relative ratio of coprostanol to 24 ethyl-coprostanol gives a profile consistent with human origin. We can exclude sheep, cow, horses, goats, dog and rabbit as the origin of these faecal stanols. We found definite lithocholic acid and a minute trace of deoxycholic acid, but no hyodeoxycholic acid in the sample. The pattern of faecal bile acids in the sample suggests that the faecal source is human and not pig.

If the sample was a mixture with adult (or juveniles on solid feed) human faeces present, then we would have expected much higher *relative* levels of the faecal stanols in the sample, so the sample is unlikely to be non-infant human faeces.

Summary

The patterns of stanols and sterols and hydrocarbons found in the sample examined are not compatible with that of human adult sewage. The alcohol/sterol fraction and hydrocarbon fraction profiles suggest that the sample examined is not material originating from a sewage treatment plant. It is unlikely that the specific location of the questioned case sample was a receptacle for sewage.

The sample examined has features consistent with having originated predominantly from decomposing remains of individuals whose diet had been predominantly vegetable oils.

In answer to the original question, the sample does show indicators which suggest that human faeces is present. However, the sample does not consist of wholly faecal material. It has not originated from a sewage treatment plant or from adult faeces.

**At the time of writing we were requested to identify the crystals in the sample by XRD (Table 2).*

Appendices

Appendix 1

Table 1 Audit Trail

MBHCOI_TM1016					
NOTE: All sample examination, description and preparation for analysis carried out in secure lab 234.					
04-Nov-16	one sample delivered by DHL Couriers.				
Date	Analyst	Sample ID	Method	Type	Hutton ID
04/11/2016	L. Dawson, J. Ross	Exhib No. LLO16 Tr 1A, Feature 1B	The sample was opened and half of the sample was transferred to a petri dish to dry. The remaining sample was retained in the original bag and stored in the fridge in lab 234.	soil	1246549
07/11/2016	L. Dawson, J. Ross	Exhib No. LLO16 Tr 1A, Feature 1B	The sample was examined and colour measured. Aretacts were removed to vial LAD1 before sieving through a 1mm sieve. The fine fraction was photographed. Coarse fraction to vial LAD2, fine fraction to vial LAD3.	soil	
07/11/2016	L. Dawson, J. Ross	LAD3	A portion of LAD3 was hand ground with an agate mortar and pestle. The ground sample was weighed out for *n*-alkane, alcohol, fatty acid and sterol analysis.	soil	
07/11/2016	J. Ross, G. Martin	LAD3	A portion of the ground sample LAD3 was given to Gillian Martin for Total Carbon analysis.	soil	
11/11/2016	J. Ross, G. Martin	LAD3	Sample LAD3 returned by Gillian Martin.	soil	
30/11/2016	L.Dawson, S. Hillier	Exhib No. LLO16 Tr 1A, Feature 1B	The sample was examined by Steve Hillier to confirm presence or absence of asbestos. Fibres were removed and given to Steve Hillier for XRD analysis (vial SH1).	fibres	

Signature... Lorna Dawson ....

Appendix 2

References

Dawson, L.A. and Hillier, S. (2010) Measurement of soil characteristics for forensic applications. *Surface and Interface Analysis*. 42, 363-377.

Dawson, LA. and Mayes, RW. (2014) Criminal and Environmental Soil Forensics, In: B Murphy & R Morrison (eds), Introduction to Environmental Forensics, 3rd Edition. Academic Press.

Munsell (2000) Soil Colour Charts. Gretagmacbeth. 617 Little Britain Road, New Windsor, NY 12553.

Thornton et al, (2015) Distributions of carbon and nitrogen isotopes in Scotland's topsoil: a national-scale study. European Journal of Soil Science. 66, 1002-1011.

Appendix 3

Glossary of technical terms

Derivatisation of compounds of interest prior to analysis by gas chromatography:
The use of **BSTFA** reagent to convert any alcohol species present in the soil 'alcohol' fractions to **trimethylsilyl (TMS) ethers** not only improves gas-chromatographic separations, but with **GCMS** allows direct identification of peaks appearing on the gas chromatogram, since the individual **TMS** compounds have distinct characteristic mass spectra. Similarly, methylation of the carboxyl groups of organic acids improves improves gas-chromatographic separations; for hydroxyacids, such as the faecal bile acids and 10-hydroxystearic acid, to get good separations and distinct mass spectra, it is necessary to both methylate the carboxyl group and silylate the hydroxyl groups on the compounds.

Gas chromatography (GC): This is a method of separating and quantifying individual components (compounds) from complex mixtures, based on differences in relative affinities for a stationary phase (usually an immobilised liquid) and remaining in a vapour phase. The sample is introduced to a column (long tube) as a vapour, which is swept along the column by flow of an inert **carrier gas** (commonly nitrogen, helium or hydrogen). In the past, most gas chromatography was carried out using *packed columns* in which the stationary phase was supported by inert particles held throughout the length of the column. Most present-day applications involve the use of *capillary columns*, in which the stationary phase coats the inside of long, narrow silica, glass or metal tubing; capillary columns have much higher resolutions. As the sample vapour passes along the column, different components travel at differing rates, leading to separation of the components into individual peaks leaving the distal end of the column. The speed of passage and degree of separation is affected by the amount of stationary phase, carrier gas flow rate and column temperature. The instrument containing the column, the **gas chromatograph**, consists primarily of a temperature-programmable oven which encloses the column. Unless the sample is a gaseous mixture, samples to be analysed are usually dissolved in a volatile solvent, and introduced by means of a syringe, either directly onto the column (e.g. *cold on-column injection*), or an injection system, heated to vaporise the sample; the sample vapours are swept on to the column by the carrier gas. The separated sample component peaks reaching the lower end of the column are sensed by a *detector*, which gives an electrical response dependent on the size of the component peak. There are a number of different types of detector, dependent upon the components being analysed. For routine analysis of organic compounds the *flame ionisation detector* is most widely used. Some modern gas chromatography columns have been designed to allow compounds of relatively low volatility to be analysed, by running at high temperatures. The plant wax compounds and sterols/stanols described in the present report come under this category.

Gas chromatography-mass spectrometry (GCMS): This is essentially conventional gas chromatography fitted with a mass-selective detector, primarily for resolution of organic analytes. The separated compound molecules eluting from the chromatography column are transferred to a vacuum chamber, where they are ionised and separated and detected according to ion mass. In the most widely used configuration (as used in the work described in this report), the analyte molecules are ionised by bombardment with an electron beam (*electron ionisation*), which breaks up the molecules to produce a number of fragment ions. By using a fixed standard electron energy (conventionally 70eV), the relative percentages of the different fragment ions result in a reproducible *mass spectrum* which, being characteristic for different individual compounds, enables the compounds to be directly identified. Since the number of ions produced for a particular compound is dependent on the amounts of compound eluting from the GC column, quantitative analysis can be carried out. Counting all of the ions produced (*total ion count*, TIC) results in a gas chromatogram which is very similar to that obtained from a conventional gas chromatograph fitted with a flame ionisation detector.

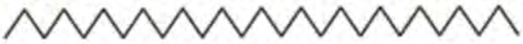
Interpretation of gas chromatograms and quantification: In conventional gas chromatography, compound peaks can be identified from the *retention time*, which is the time after injecting the sample that the summit of the peak occurs; standard mixtures containing compounds of interest also need to be run under identical conditions (temperature, gas flow rate etc.) of the gas chromatograph. Peak sizes are usually determined in terms of peak areas, determined with specialist software built into a computing integrator or computer attached to the gas chromatograph. The accurate assessment of peak area is very much dependent on the correct positioning of baselines executed by the software; this is particularly important in situations where peaks may not be fully resolved.

The *n*-alkanes, fatty alcohols, sterols and stanols in the samples analysed in this report could be quantified by adding a known amount of relevant *internal standard* compound to the sample prior to extraction, purification and analysis. Ideally, a suitable internal standard compound should not be present in the samples, but have the same physical and chemical properties as the compounds being quantified. Ideally, a suitable internal standard compound should not be present in the samples, but have the same physical and chemical properties as the compounds being quantified. It has been shown that the concentrations of the chosen internal standards for *n*-alkanes and for fatty alcohols can be considered as having negligible concentrations in plant and soil samples. The internal standard used to quantify *n*-alkanes was tetratriacontane (C34).The fatty alcohol internal standard was1-heptacosanol (C27-ol), the fatty acid standard was hentriacontanoic acid (C31) and 5β-cholan-24-ol was added as the internal standard for the sterols and stanols.

ORGANIC MARKERS RELEVANT TO THIS REPORT

Plant wax compounds: Lipid (hydrophobic) compounds found in the surface wax of plants. These can be complex mixtures. The plant wax compounds mentioned in this report are listed as follows:

***n*-Alkanes**: straight-chain, C_{21}-C_{37}, with odd-chain compounds predominating



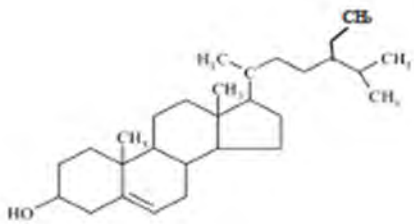
Primary long-chain fatty alcohols: straight-chain, C_{20}-ol - C_{34}-ol, predominantly even-chain

Sterols and stanols:

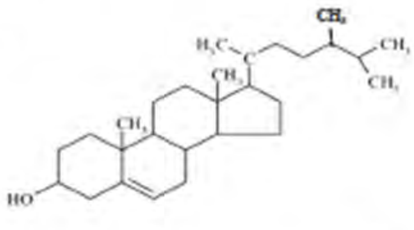
These, if present, occur in the 'alcohol' fraction eluted from silica-gel columns. Sterols are unsaturated (i.e. containing one or more double bonds) steroidal alcohols; stanols are saturated steroidal alcohols.

Sterols:

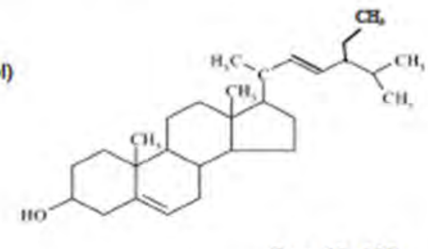
β-Sitosterol (24-ethyl cholest-5-en-3β-ol):
main sterol found in plants



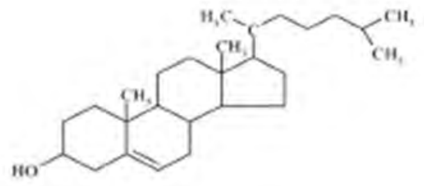
Campesterol (24-methyl cholest-5-en-3β-ol):
common plant sterol



Stigmasterol (24-ethyl 5,22-dien-cholestan-3β-ol)
common plant sterol

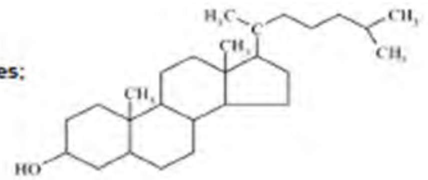


Cholesterol (cholest-5-en-3β-ol):
main sterol found in animals



Stanols:

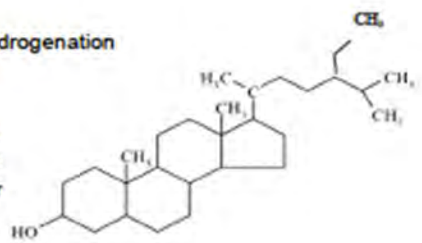
Coprostanol (5β-cholestan-3β-ol): hydrogenation product of cholesterol occurring in mammalian faeces; main stanol in human and pig faeces



Epicoprostanol (5β-cholestan-3α-ol): isomer produced from coprostanol by microbes under anaerobic conditions (e.g. septic tank)

Cholestanol (5α-cholestan-3β-ol): another isomer produced by hydrogenation of cholesterol under anaerobic conditions in the environment (not in the mammalian gut).

24-Ethylcoprostanol (24-ethyl 5β-cholestan-3-β-ol): hydrogenation product of β-Sitosterol; main stanol in herbivore faeces



24-Ethyl epicoprostanol (24-ethyl 5β-cholestan-3α-ol): isomer produced from 24-ethylcoprostanol by microbes under anaerobic conditions (e.g. farm slurry tank); minor stanol in fresh faeces

Stigmastanol (24-ethyl 5α-cholestan-3β-ol):
another isomer produced by hydrogenation of β-sitosterol under anaerobic conditions in the environment (not in the mammalian gut

Campestanol (24-methyl 5α-cholestan-3β-ol): hydrogenation product produced by hydrogenation of campesterol under anaerobic conditions in the environment (not in the mammalian gut).

NB: The structural diagrams of the above stanols and isomers are generic. The numbers refer to the individual carbon atoms within the steroidal structure and the Greek letters (α and β) refer to whether the side group (e.g. the 'OH' group) is in a position above or below the ring structure. The same applies to 24-ethylcoprostanol, campestanol and their isomers.

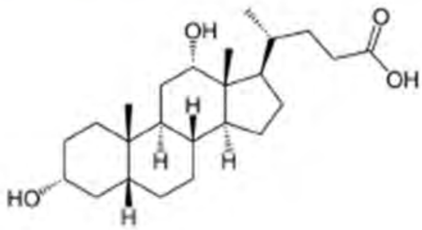
Signature... Lorna Dawson ....

Faecal bile acids:

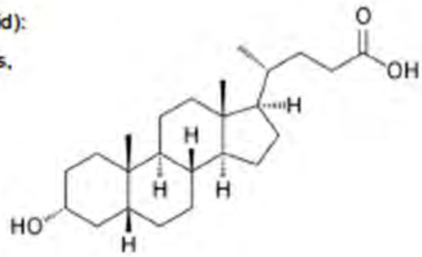
Bile acids are steroidal hydroxyl acids. The compounds of interest as markers found in faeces are secondary bile acids, which have been transformed by gut bacteria from primary bile acids (cholic acid and chenodeoxycholic acid) which had been secreted into the gut from bile.

Lithocholic acid (3α-hydroxy-5β-cholan-24-oic acid):

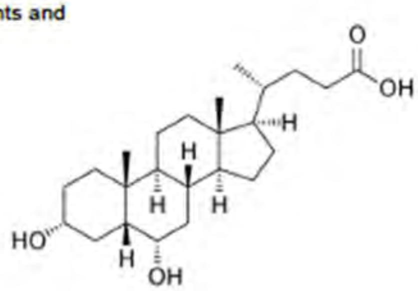
found in faeces of most mammals, including faeces from humans, pigs, ruminants and other herbivores.



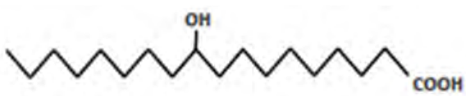
Deoxycholic acid (3α,12α-dihydroxy-5β-cholan-24-oic acid):
found in faeces of humans, ruminants and other herbivores, but not in pig faeces



Hyodeoxycholic acid (3α,6α-dihydroxy-5β-cholan-24-oic acid):
found in pig faeces, but not in faeces of humans, ruminants and other herbivores



10-Hydroxy stearic acid:



Produced from oleic acid by microbes under wet anaerobic conditions. It is a major constituent of adipocere, which is a white soapy substance originating from body fat and found in cadavers which had decomposed in a waterlogged environment. 10-Hydroxystearate is thus a useful body decomposition marker. It has also been found in human faeces.

Other terms used in this report:

Mineral - A mineral is a naturally occurring solid chemical substance, formed through geological processes, which has a characteristic chemical composition, a highly ordered atomic structure, and specific physical properties consequent upon its structure and chemistry.

Organic - Pertaining to a class of chemical compound that exist in or have been derived from plants or animals.

Appendix 4

Summary of procedure for the analysis of soil samples for organic lipid markers

High-purity solvents are re-distilled (*n*-heptane, ethanol and ethyl acetate) before being used.

The air-dried soil samples were hand milled in an agate mortar and pestle. Duplicate sub-samples of each soil (about 200mg) were weighed with alkane,fatty alcohol and sterol internal standard compounds from separate solutions of known concentration (C22 and C34 *n*-alkanes, C27 alcohol and 5β-cholan 24ol, respectively) into screw capped tubes with PTFE cap-liners, and heated overnight in sealed screw-cap vials with 1M ethanolic KOH at 90°C.

After cooling to 50°C and the addition of water, any hydrocarbons (including *n*-alkanes) and alcohols present were extracted twice with *n*-heptane. After removing the solvent, the heptane extracts were re-dissolved in heptane prior to being transferred to a small glass solid-phase extraction column packed with about 50mg of silica-gel. The hydrocarbons were eluted from the column with *n*-heptane. The solvent was then changed to 20% ethyl acetate/ 80% *n*-heptane (v/v) in order to elute any fatty alcohols, sterols and triterpenols (crude alcohol extract). The hydrocarbon extract was dried and redissolved in dodecane prior to analysis by GC. The crude alcohol extract was derivitised with a mixture of BSTFA and pyridine before drying and redissolving in dodecane prior to analysis by GC-MS.

The residue remaining after alkane and alcohol extraction was acidified and extracted with chloroform. The extracted compounds were added to an SPE column containing aminopropyl packing. The organic acids were eluted with a mixture of diethyl ether and glacial acetic acid. After drying the acids were converted to their methyl esters, by heating with acidified methanol and then further treated with BSTFA to silylate the hydroxyl groups (as trimethylsilyl ethers on hydroxy acids). The derivatised extracts were analysed by GCMS in TIC mode.

Appendix 5

Images of soil examined

Photographs of soil sample examined (fractions which passed through a 1mm sieve). (Scale = mm)

Plate 1 Sample from Feature 1 (<1mm sieved) at X20 magnification

Plate 2 Feature 1 Soil aggregates and white material at X40 magnification.

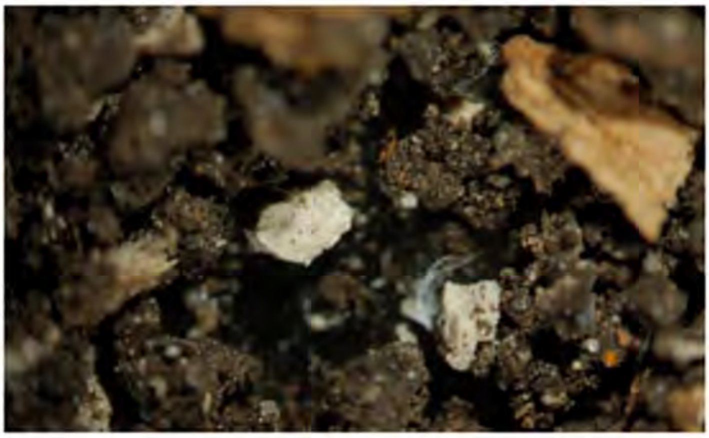
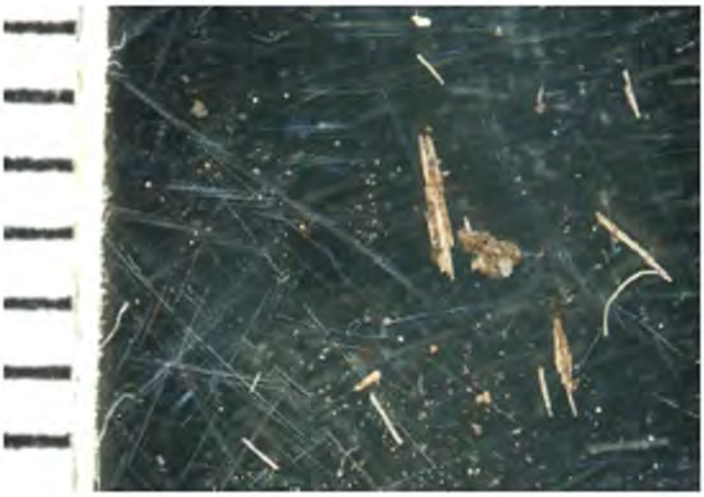


Plate 3 Feature 1 Fragment of bone at X40 magnification.

Plate 4 Feature 1 Fibres removed for X-ray Diffraction (XRD) analysis



31st May | 2017

Directed Site Investigations at the reported *'Children's Burial Ground'*, Dublin Road Housing Estate, Tuam, Co. Galway: Results of Phase IIA

Report to The Mother and Baby Home Commission of Investigation

Niamh McCullagh, MA MSc MCSFS
Forensic Archaeologist, Project Director

Aidan Harte, BA MA MIAI ACSFS
Senior Archaeologist, GIS Specialist

Linda Lynch, MA PhD MIAI
Human Osteoarchaeologist

Contents

List of Tables

EXECUTIVE SUMMARY

- This excavation was completed to forensic standards and within the parameters requested by the Mother and Baby Home Commission of Investigation.

- This investigation (Phase IIA) was an extension of Phase II and was designed to expose the extent of Feature 1, the chambered tank structure identified in 2016.

- A further 16 chambered tanks were exposed bringing the total to 20 individual chambered tanks along the extent of Feature 1.

- The base of Feature 1 is approximately 2.70m below the present ground surface, was not accessible and thus, was not forensically examined as part of this phase of works.

- The structural nature of Feature 1 limited investigations to visual observation and soil sampling.

- Each chamber has an opening at the top. Eight chambers have clearly defined openings at the base, with more indistinct breaches at the base in others.

- It is highly likely that this structure was originally constructed for the treatment of sewage waste.

- Juvenile human remains, in significant quantities, were observed in 18 of the total 20 chambers.

- Juvenile human remains observed were in an excellent state of preservation.

- Evidence exists that supports potential articulation of these remains at the time of interment.

- Osteological observations support the age range representing of individuals being infant, less than 1 year of age, and young juvenile, from 1-6 years of age.

- Archaeotanathology indicates there have been significant fluctuations of the water-table within the individual chambers.

- Soils analysis indicates the presence of the biomarkers of human sewage and human decomposition products within the chambered tanks, however the timing of when these activities occurred cannot be ascertained.

- A decision on the future of the site needs to be made as soon as possible to prevent potential damage to the remains that lie there. There is a risk of disruption to preservation of context, articulation evidence and the preservation of DNA. While this threat is not necessarily immediate it does exist.

- It is not appropriate to leave juvenile human remains in this specific context.

1. Introduction

This report presents the results in full of an extension of site investigation work carried out at the site of the reported 'Children's Burial Ground' at the Dublin Road Housing Estate, Tuam, Co. Galway in November 2016. This further excavation was undertaken on behalf of the Mother and Baby Home Commission of Investigation, herein MBHCOI, with the cooperation of An Garda Síochána, and represents Phase IIA of site investigations.

A significant sub surface feature, Feature 1, was identified in Phase II. This required further investigation on behalf of the MBHCOI in order to establish its full extent and if further human remains are present. Niamh McCullagh, Forensic Archaeologist, directed all works on-site for the duration of Phase IIA.

This report presents the methodology, the results in full, including human remains, artefacts recovered, and soils analysis. Finally the condition of the site post excavation is described. The scale and significance of findings in Phase IIA further highlights the requirement that careful and swift consideration is undertaken to decide upon the future of human remains at the site.

1.2 Aims and Objectives of the Excavation

This excavation took place at the request of the MBHCOI, under the Commissions of Investigation Act 2004, Sections 8, 26 and 28. This additional excavation was undertaken under the same warrant that had been issued on the 1st of September 2016 by Judge Yvonne Murphy, in accordance with Section 26 of the Commission of Investigations Act 2004. This warrant authorised Niamh McCullagh to exercise the powers given under Section 28 of the Act in relation to premises known as the Children's Burial Ground located in the Dublin Road Housing Estate, Tuam, Co. Galway, see **Appendix I**.

On the 13th of December 2016 the MBHCOI requested specifically that the structure identified as Feature 1 in Phase II be exposed completely and investigated further. This phase was designed to be an non-intrusive investigation, with observations to be made on the contents of each chamber and a contemporaneous photogrammetric record be made. No human remains were to be recovered during this phase. An additional request was made for soil sampling to be undertaken whilst on site to inform the MBHCOI regarding the potential the chambers had been used for the storage of sewage. No other areas of the site were disturbed during the course of this work.

The matters requiring investigation for Phase IIA were:

i. To establish the extent of the previously identified feature, Feature 1, found in Phase II.
ii. To establish if there were further human remains at this location.
iii. To conduct a comprehensive soil sampling exercise in order to detect if Feature 1 had been used to store human sewage.

A controlled forensic excavation, focused on Feature 1, took place from the 30th of January to the 10th of February 2017. Additional analysis was conducted post-excavation amounting to a further three months in duration to bring the project to the production of report.

1.3 Test Excavation

As the MBHCOI could not justify a full excavation at this point, the investigative strategy that was utilised for Phase IIA is what is termed a 'test excavation' approach. This method uses focused trenches rather than open area excavation and is designed to have minimum impact on the site while allowing relevant evidence to be recovered. The three concerns of the Commission were to be addressed by conducting this test trench method of excavation over the structure Feature 1. This ensured that the remainder of the site was undisturbed and available for future investigations.

1.4 Forensic Archaeology

The site investigation required a full forensic control to be in place and to direct works on site; this is due to the modern nature of the site and the modern context of expected results. Niamh McCullagh, as a suitably qualified and experienced Forensic Archaeologist, was appointed this task.

The timeframe under consideration was from 1925-1961, the duration of the operation of the Mother and Baby Home associated with this site. The modern nature of the site gave rise to the potential for it to become regarded as a crime scene. All evidence collected is required to be of a standard submissible in a criminal court of law, that is, to the evidential standard that is required by forensic cases.

In traditional archaeology the emphasis is generally on a cultural interpretation of the past, as opposed to specific, individual events. Standards of evidence and interpretation are not subjected to the scrupulous standards required by a court of law. While methods used are similar the interpretations are not, neither are the forms of evidence gathered.

In adherence with best practice, manual archaeological excavation conformed to the Museum of London Archaeological Standards (MoLAS) and the codes of practice of the Institute of Archaeologists of Ireland (IAI). This meant documentation through single context archaeological recording, by written descriptions, scaled photographs, and surveyed drawings. The written descriptions of soils, scaled photography, and scaled section and plan drawings (at 1:10 and 1:20), were archived by register on-site – a practice referred to as preservation by record. In this case, for management of space, the void that was created by the construction of each chamber was also given a context number. The contents of each chamber were further recorded through the use of rendered photogrammetry. A detailed record of the archaeological site work undertaken has been retained and the site archive is available on request.

Forensic archaeological standards were maintained in accordance with the 'Standards and Guidance for Forensic Archaeologists' (Powers and Sibun, 2011), prepared for the Chartered Institute for Archaeologists, UK, and the Handbook of Forensic Anthropology and Archaeology (World Archaeological Congress Research, 2011), Blau, S. & Ubelaker, D. (eds). Please see technical note in **Appendix II** for further details.

1.5 Methodology for Phase IIA

The investigative strategy utilised for this investigation was similar to the 'Test Excavation' approach, which has the minimum impact on the site while allowing relevant evidence to be recovered. This protects the integrity of the human remains and the deposition site.

The excavation design consisted of placing a single trench directly over the area of interest. The location and size of this single trench was informed by the results of the desktop review, the geophysical survey conducted (Utsi, 2015), the initial test excavation (McCullagh, 2016), and as requested by the Mother and Baby Home Commission of Investigation. This excavation had a high potential to reveal further human skeletal remains, hence all work ensured that any such remains were treated with the utmost dignity and respect while maintaining forensic protocol.

The excavation methodology for Phase IIA was conducted as per the proposal for Phase II dated 10th August 2016. Forensic control was maintained throughout the site investigation. All mechanical works were monitored by archaeological personnel and all manual excavation was undertaken by qualified archaeological personnel. The site investigation was implemented in the following stages:

1. The location of the chambered structure was identified on the surface of the site.
2. Topsoil and gravel, the overburden, was removed using a track machine fitted with a grading bucket (3 Tonne) under archaeological supervision. This was carried out in two stages; initially the Western extent of Feature 1 was exposed followed by the Eastern extent of the chambered structure.
3. Once overburden was removed, manual excavation by archaeologists exposed the fractured lids or coverings over each of the chambers identified and an appropriate record was made prior to the next stage.
4. Each of these lids was then removed and the internal structure and contents were assessed and appropriately recorded.
5. A temporary timber covering was placed over each opening for the duration of works on site.
6. The extent of the opened trench was covered by commercial marquee for the duration of works.

Any human remains uncovered on site whilst being of evidential value, were treated with dignity and respect. As the extent of Feature 1 was uncovered, each chamber was covered as work progressed (unless that chamber was being recorded at that the time). Once excavation was underway the trench was protected by a commercial marquee that acted as a scene tent to shelter sensitive evidence, to prevent overlooking, and keep the open trenches safe, **Appendix III Plate 1.1.**

A number of additional measures were put in place to protect the integrity of the site and in respect of the sensitivity of such a project. The site was surrounded by plywood hoarding to inhibit line-of-sight and to offer security to the location and to staff for the duration of works. Security of the site was also maintained throughout the excavation by the 24/7 presence of An Garda Síochána.

2. Results of Excavation

2.1 Structural Evidence

Aidan HARTE and Niamh McCULLAGH

Feature 1 (C.5 etc.) can be clearly seen depicted in the geophysical results, see **Appendix IV Figure 2.1 FIGURE**. The layout drawing illustrates the archaeological features as uncovered during excavation. Overlain are the interpreted extensions of those masonry features, as identified from the geophysical survey. The latter has been re-worked to reflect the actualities of the archaeological remains.

2.2 Nineteenth Century Cesspit

These results alter the extrapolated measurements of the overall cesspit as calculated in Phase II. Consequently, the cesspit likely measures 11.16m x 8.02m internally. Note that the northeastern corner is not clear in the geophysical survey. This may be the result of infill of the cesspit originating from this location but may also highlight further masonry features in this direction. The internal rectangular feature within the cesspit at north (i.e. Feature 2) does not form a clear anomaly in the magnetometry/gradiometry survey results (Utsi, 2015). It is therefore possible that further divisions of the original cesspit exist but cannot be coherently mapped from the geophysical survey alone.

2. 3 Feature 1

The focus of this investigation was on Feature 1, see **Appendix IV Figure 2.2** for site matrix. Feature 1 may generally be described as a later addition within the 19^{th} Century workhouse cesspit that had been located during Phase II. It consists of stone walls, shuttered with concrete, utilising the southern end of the earlier cesspit. The stone and mortar constructed southern wall of the cesspit and southernmost 1.6m of both the East and West walls of the cesspit, form boundaries of Feature 1. This is clearly visible internally to C. 50/52 and C.104/105 and in places along the length of the southern wall where the concrete shuttering has not been placed on the pre-existing wall e.g. C. 71, C.75, C.73, indicating the time frame and sequence of construction that occurred here.

2. 3. 1 Openings

Within the separate tanks that form Feature 1, a number of observations can be made. Without exception, all tanks have access through an opening at the top of the tank, C. 5. There are 21 openings that correspond to 20 internal chambers; C.50, C.52, C.54, C.56, C.58, C.60, C.62, C.64, C.82, C.84, C.86, C.88, C.90, C.92, C.94, C.96, C.98, C.100, C.102 and C.104, see **Appendix III Plates 2.1 & 2.2**. The size of the openings at the top of each tank is essentially identical; each opening averages 0.84m in length (minimum 0.82m and maximum 0.85m), and averages 0.29m in width uniformly. This further supports the view that timber formwork was used in the construction of the concrete cap closing the tank; see **Appendix IV Figure 2.3 & 2.4 and Appendix III Plates 2.3.**

2. 3. 2 Lids/Covers

A lid had covered each of the 21 openings. Lids believed to be the original lids are of similar construction and material as the concrete capping, **Appendix III Plates 2.4**. These were pre-cast concrete, approximately 6cm in thickness. A number of these had been broken and replaced throughout the history of use of the chambers. In some instances, although fractured, most of the original lid was found covering the opening. Most repairs or replacements were found at the northern half of each opening. While in some cases materials such as corrugated steel was used, it was more commonly outsized crude concrete slabs that replaced broken portions of lids **Appendix III Plates 2.5 & 2.6.** In the case of C.86/87 the covering lid had completely degraded and soil compaction was all that remained over the opening.

2. 3. 4 Internal openings

All further noted breaks, gaps and openings are at the base of the northern wall within each tank. These openings are well-defined in the eight easternmost chambered tanks. The first tank on the eastern end (C.50) has a squared opening to north, estimated between 0.25m - 0.31m in width. This opening extended through the wall to north where it had been closed using a metal cover. This may have been unintentional but does provide a clarity on the construction of the opening. It seems that the opening was shuttered with concrete, using formwork, during the construction of the north wall. The position at which it enters the chambered tank is slightly off-centre to the west.

The next chambered tank to the west, C.52, has a squared opening that has been blocked with debris which had seemingly originated at north. It has an estimated width of approximately 0.36m and is off-set significantly to the west of centre. The internal face of the north wall here has an observable kink, whereby the footing appears to have been stepped back, by as much as 80mm.

Tank C.54, the next chamber to the west, again has a squared basal opening. Although some debris is present within the opening, it is clearly defined, with an estimated width of 0.37m, centrally positioned in relation to the tank. The basal opening in the next tank to the west, C.56, is again squared with an approximated width of 0.34m. Notably, this opening is displaced to the east of the tank, so much so that the eastern dividing wall appears to have been recessed to accommodate it. Chambered tank C.58, to the west, again has a squared opening at the base. This is also heavily displaced to the east and has an estimated width of 0.32m. Further west, chambered tank C.60, has a squared opening at the base between 0.3m and 0.32m in width. Debris has partially filled the opening which is set slightly off-centre to east.

The opening at the base of the chambered tank to the west, C.62, is particularly interesting in that it has been largely blocked from the far side (north) by large pieces of limestone and mortar. This has preserved some of the timber form-work at the head of the opening. It is 0.36m in width and very slightly off-set to the west. Finally, the next chambered tank to the west, C.64, has a basal opening measuring between 0.38m – 0.4m and is positioned almost flush with the eastern wall of the chamber. The eastern wall of the chamber appears to lean eastwards as it rises.

These formal openings, all occur in the north wall and at the eastern end of Feature 1. Where most clearly evident (C.58, C.62 and C.64), the height is greater than the width of the openings. The depth of each opening is that of the thickness of the wall but in most instances debris has been displaced through the openings from north.

The position of the openings, relative to the tanks is interesting, as it suggests that the northern wall – and its openings - was constructed before the internal dividing walls. However, seemingly no further deliberate openings were made along the remaining section of northern wall to the west. It is worth noting that breaks, gaps or other breaches in the north wall are evident in most of the other tanks to the west, with the exception of the westernmost end tank C.104. These breaches in the western half of the north wall are most substantial in tanks C.84, C.86, C.88, C.94 and C.96.

Chambered tank C.84 is interesting due to the fact that though there is a crude breach at the base of the wall, the shuttered concrete above suggests that a squared opening had been constructed but was subsequently filled in and shuttered over. The regular form of other breaches may also be resultant of a similar construction. At chambered tank C.88 the breach is very regular except for at the top and at C.94 it appears stones may have been used to fill the opening and were then crudely concreted over. Alternatively, the creation of these breaches (i.e. through hydraulic erosion) has removed sections of the regularly coursed masonry found within an otherwise homogeneous wall. Nevertheless, it is clear that the base of the northern wall of Feature 1 has deliberate openings at the eastern end and is similarly breached at many points along the remainder.

In every chambered tank, the south wall is limestone and mortar construction. At the end tanks (C.50 and C.104) the end walls are of the same construction and extend beyond Feature 1 to the north. This southern wall is therefore the original cesspit wall. The northern wall appears to have been constructed to separate a rectangular space which was to be divided into 20 voids/tanks.

2. 4 Discussion

The purpose of this structure remains largely unclear but it does seem plausible that each chambered tank was expected to act as a cesspool. A 'cesspit' is a place/tank in which waste material collects and is emptied manually at intervals, while 'cess pool' by definition is a place in which waste is deposited but allowing the liquid part to percolate into the surrounding soil.

A septic tank, by contrast, necessitates the filtration of all material so that solid waste is broken-down before percolating elsewhere. It is possible that the eight eastern tanks were designed to act at cesspools, liquids percolating into the former cess pit to the north. However, during the course of construction, this design template may have been abandoned, opting instead for simple cess pits that were not to be emptied. It must be understood that this would have been a very short term out-look for any sanitation project.

The cast concrete cap (C.5) was created *in-situ*. The basal timbers of the casting boards are still in place in some instances (most notable at C.62)**, Appendix III Plate 2.7,** and much of the timber debris within the tanks may have originally been part of this. Also of interest is tank C.102, which has a low dividing wall in the interior, while C.82 immediately to the west has two openings at the top. It is likely this was done in error and that the double openings of C.82 were in fact meant to access two separate tanks at C.102. Following the cast, the internal wall of C.102 was reduced in height.

3. Human Remains Evidence

3.1 Human Remains Evidence and Analysis

Dr Linda G. LYNCH

This report details the osteoarchaeological assessment of the photographic record of the most recent investigations (Phase IIA) by the Mother and Baby Homes Commission Of Investigation (MBHCOI) of the site at Tuam. Previous test excavations identified juvenile (<18 years) human skeletal remains within, and to the exterior (north) of, four underground tanks associated with a larger concrete structure (McCullagh 2016).

3. 2 Methodology

Unlike the initial test excavations in Phase II, no skeletal remains were recovered during the most recent archaeological investigation (Phase IIA). The surfaces of the deposits in the 16 tanks were almost 2m below the upper capped concrete surface. Photogrammetry was undertaken, which enabled the whole surface of each deposit to be photographed in detail. Human skeletal remains were identified in 14 out of the 16 tanks exposed during this investigation.

A composite photograph of each tank was processed by A. Harte for planning purposes. These composites are used in this report as the base photograph of each chambered tank, which are examined separately below. Each composite photograph is annotated (in terms of skeletal remains), and more detailed descriptions of identified, and unidentified, human remains is provided, including more specific photographs. In some cases, it was possible to identify individual bones. While every group of bones, or actual identifiable bones, are indicated in each tank, not every single fragment of bone is highlighted.

No adult bone (18+ years) was identified, and all identifiable skeletal remains within the tanks appeared to be from either infants (<1year) or young juveniles (1-6 years). It was not always possible to correctly identify the age group and many bones are simply classed as juvenile – in this instance 'juvenile' specifically refers to individuals aged 6 years or less at the time of death.

A number of instances of possible articulated human skeletal remains were identified on the surfaces of the sediments within the tanks. However, this does not necessarily indicate *in situ* remains. It appears likely that there has been considerable fluctuation in water levels in the tanks since the human remains were originally deposited, resulting in a redistribution of skeletal elements. This will be further examined in the discussion.

As a reference guide to the photographs and text, where some technical language is used, there are diagrams of the main bones of the human skeleton, the main elements of the infant cranium, anatomical directions, and a glossary of osteoarchaeological terms in Appendix VI, A-D.

3. 3 Human Skeletal Remains (as determined from photographic analysis)

In total, 16 additional tanks were opened during the present investigation. Human skeletal remains were identified in 14 of them. In most of the photographs, north is always to the top, unless otherwise stated.

C.50/51

This is the easternmost tank of Feature 1. It was identified in Phase II and reported on in full (see McCullagh 2016)

C.52/53

This tank is immediately to the west of tank C.50/51. It comprises a single narrow chamber. **Appendix III Plate 3.1** is a general annotated photograph of the base of the tank, while **Appendix III Plate 3.2** to **3.7** show the identified elements in more detail. Human remains were identified on the surface of the sediment, at the north end of the tank (a), along the eastern side (b) and (c), and at the southern end (d).

The identified human remains are summarised in **Table 3.1**.

Location as indicated in primary photograph Plate 3.1	Details	Plate reference (see Appendix III)
a	Multiple cranial remains of infants (<1 year) and/or young juveniles (1-6 years)	3.2
b	Collection of possible infant (<1 year) remains including two separate sets of possible articulated ribs, and other possible indicators of articulation	3.3
c	Infant (<1 year) cranial fragment and long bone	3.4
d	Multiple possible infant (<1 year) remains including two individual sets of possibly articulated ribs and two mandibles	3.5, 3.6, 3.7

Table 3.1: Identified human skeletal remains within tank C.52/53

A collection of primarily cranial remains is present at the northern end of the tank (see **Appendix III Plate 3.2**), which may be from either infant/s (<1 year) and/or young juveniles (1-6 years). It is possible that multiple individuals are represented here. There is some suggestion of articulation in the bones indicated in **Appendix III Plate 3.3**, located along the east side of the tank, which appear to comprise infant remains (<1 year). At least two separate concentrations of ribs appear in an articulated state, while a possible left humerus and ulna (upper arm and forearm bones) are in the approximate location for being articulated. It may also be more that coincidence that there are two tibiae (shin bones) close together. There also appears to be a concentration of possible infant vertebrae.

A possible infant cranium and long bone was identified along the middle of the eastern side of the tank (see **Appendix III Plate 3.4**).

At the southern end of the tank a significant concentration of skeletal remains was identified (**Appendix III Plate 3.5**). Two individual sets of possibly articulated possible infant ribs were identified. In addition to a large concentration of possibly infant/young juvenile cranial remains, ribs, and long bones, two mandibles were identified. The first mandible (**Appendix III Plate 3.6**) is probably from an infant <1 year at the time of death. Another probable infant mandible (<1 year) was also identified (**Appendix III Plate 3.7**).

C.54/55

This tank was immediately to the west of tank C.52/53. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.8** is a general annotated photograph of the base of the tank, while **Appendix III Plates 3.9-3.13** show the identified elements in more detail, while other information is detailed in **Appendix III Plates 3.14** and **3.15**. Human skeletal remains were identified in the southern half, (a) and (b), of the tank.

The identified human remains are summarised in **Table 3.2**.

Location as indicated in primary photograph Plate 3.8	Details	Plate reference (see Appendix III)
a	Various infant (<1 year) and/or young juvenile (1-6 years) remains	3.9, 3.10
b	Infant/young juvenile cranial remains (<6 years), adjacent to animal bone, with an infant (<1 year) femur and associated possible hand bones suggesting some possible articulation	3.11, 3.12, 3.13

Table 3.2: Identified human skeletal remains within tank C.54/55

Infant (<1 years) and/or young juvenile (1-6 years) skeletal remains were identified just to the south of the middle of the tank (see **Appendix III Plate 3.9**). There was no evidence of articulation.

An infant femur (thigh bone) and hand bones were identified in the northern end of the tank (**Appendix III Plate 3.11**), which may suggest some degree of articulation (**Appendix III Plate 3.12**). In addition, cranial remains of an infant were identified underlying what appears to be a large animal bone fragment in the southwest corner of the tank (**Appendix III Plate 3.13**).

Two small possible fragments of human bone were tentatively identified attached to the north-facing wall of the tank (**Appendix III Plate 3.14**).

A possible piece of wickerwork (**Appendix III Plate 3.15**) was identified at the northern end of the tank (see **Appendix III Plate 3.8** for location).

C.56/57

This tank was immediately to the west of tank C.54/55. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.16** is a general annotated photograph of the base of the tank, while **Appendix III Plate 3.17** to **3.23** show the identified elements in more detail. Skeletal remains were identified at the northern end of the tank (a), near the centre (b), and in the southern half (c) and (d).

The identified human remains are summarised in **Table 3.3**.

Location as indicated in primary photograph Plate 3.16	Details	Plate reference (see Appendix III)
a	Multiple infant (<1 year) and/or young juvenile (1-6 years) cranial bones	3.17
b	Infant (<1 year) and/or young juvenile (1-6 years) cranial bone	3.18
c	Multiple possible infant (<1 year) long bones	3.19
d	Cranial remains of at least two young juveniles (1-6 years), as well as other skeletal remains	3.20, 3.21, 3.22, 3.23

Table 3.3: Identified human skeletal remains within tank C.56/57

Multiple infant/young juvenile bones (that is, <6 years) were evident in the areas marked (a), (b), and (c) in **Appendix III Plates 3.17-3.19**. In **Appendix III Plate 3.17**, a thoracic vertebral arch of a young juvenile (1-6 years) is also visible.

Multiple juvenile cranial fragments were present at the southern end of the tank and some of these are indicated in **Appendix III Plate 3.20**. At least two young juveniles (1-6 years) appear to be present. On the right side of the photograph is the occipital squama (back of skull) and right temporal (side of skull) of a possible young juvenile (1-6 years). The other left and right temporals, occipital squama and pars lateralis, and pars basilaris, in the main area of the photograph, are probably all from another juvenile individual. These bones form the sides, back, and base of the skull. The pars lateralis appear at least partially fused to the squama, which typically occurs between 1-3 years of age (after Schaefer et al. 2009, 15). The pars basilaris is completely separate: this typically fuses to the pars lateralis between the ages of 5-7 years (ibid.).

Some additional skeletal remains were identified in the southern end of the tank and these are specifically highlighted in **Appendix III Plate 3.21-3.23**. A set of infant/juvenile ribs were visible along the west-facing wall, which may suggest some degree of articulation (**Appendix III Plate 3.21**). The mandibular remains of a young juvenile were also evident in this area (**Appendix III Plate 3.22**). It is tentatively suggested that the first and second deciduous molars may have been erupted at the time of death which would indicate an individual aged between approximately 2-4 years at the time of death. A probable young juvenile (1-6 years) thoracic arch is visible adjacent to the mandible. Finally, there was a concentration of possible juvenile ribs and vertebrae (**Appendix III Plate 3.23**) near the southeast, which may suggest some articulation.

C.58/59

This tank was immediately to the west of tank C.56/57. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.24** is a general annotated photograph of the base of the tank, while **Appendix III Plate 3.25-3.32** show the identified elements in more detail. Human skeletal remains were identified in the northern half (a) and in the southern half, (b) and (c).

The identified human remains are summarised in **Table 3.4**.

Location as indicated in primary photograph Plate 3.24	Details	Plate reference (see Appendix III)
a	Numerous possible infant remains, with some possible articulation	3.25, 3.26, 3.27
b	Possible infant hand bones, possible infant/young juvenile articulated vertebrae and ribs	3.28, 3.29, 3.30
c	Infant bones	3.31

Table 3.4: Identified human skeletal remains within tank C.58/59

A large amount of human skeletal material was evident at the northern end of the tank (**Appendix III Plate 3.25**), with multiple cranial possible infant bones evident, as well as various bones of the limbs and a pelvic bone (**Appendix III Plate 3.26**). A possible infant ulna and radius were tentatively identified which may be in an articulated state (**Appendix III Plate 3.27**).

Other possible infant bones were also identified on the east side of the tank (see **Appendix III Plate 3.24-3.28**). Possible infant hand bones were identified (**Appendix III Plate 3.29**): the fact that they are adjacent is suggestive of some degree of articulation. More convincing evidence of articulation was evident in a set of possible infant/young juvenile thoracic vertebrae and left ribs (**Appendix III Plate 3.30**). In the latter, the medial ends of the ribs appear to be in the general position for articulation with the left transverse process of at least two thoracic vertebrae. This could also be a young juvenile individual. Finally cranial and rib remains from a possible infant were also identified (see **Appendix III Plates 3.31**).

In addition to the skeletal remains evident in the sediment, an infant/young juvenile hand phalanx was identified attached to the concrete cladding of the tank in the northwest corner (**Appendix III Plate 3.32**). This was located above the extant sediments.

Finally, the remains of a black, probably plastic, hair comb (**Appendix III Plate 3.33**) were identified near the northern end of the tank (see **Appendix III Plate 3.25** for location).

C.60/61

This tank was immediately to the west of tank C.58/59. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.34** is a general annotated photograph of the base of the tank, while **Appendix III Plate 3.35-3.37** show the identified elements in more detail, while another detail is shown in **Appendix III Plate 3.38**.

The identified human remains are summarised in **Table 3.5**.

Location as indicated in primary photograph Plate 3.34	Details	Plate reference (see Appendix III)
a	Multiple infant (<1 year) and possible young juvenile (1-6 years) bones	3.35, 3.36
b	Infant bones (<1 year)	3.37

Table 3.5: Identified human skeletal remains within tank C.60/61

Infant and possible juvenile cranial fragments, and other bones, were evident at the northern end of the tank (**Appendix III Plate 3.35-3.36**), while infant bones were present at the southern end (**Appendix III Plate 3.37**).

A piece of timber on the western side of the tank, near the southern end (**Appendix III Plate 3.38**) appeared quite angled. It is possible that this may have been deliberately shaped and is suggestive of a coffin.

C.62/63

This tank was immediately to the west of tank C.60/61. It comprised a single narrow chamber. No human skeletal remains were identified in the deposits. **Appendix III Plate 3.39** provides a composite image of the surface of the sediments.

C.64/65

This tank was immediately to the west of tank C.62/63. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.40** is a general annotated photograph of the base of the tank, while **Appendix III Plates 3.41** and **3.42** show the identified elements in more detail. The human remains, (a) and (b), appear to be confined to the northern half of the tank.

The identified human remains are summarised in **Table 3.6**.

Location as indicated in primary photograph Plate 3.40	Details	Plate reference (see Appendix III)
a	Possible infant (0-12 months) cranial bone	3.41
b	Possible infant possible petrous portion (part of temporal bone of cranium) and another possible bone fragment	3.42

Table 3.6: Identified human skeletal remains within tank C.64/65

A fragment of a possible infant cranium is clearly visible at the northern end of the tank (area marked (a) in **Appendix III Plate 3.40**, see **Appendix III Plate 3.41**). In the area marked (b) in **Appendix III Plate 3.40**, the identification of the possible petrous portion (**Appendix III Plate 3.42**), is also tenuous: in some photographs it more closely resembles a piece of timber while it others it appears to resemble a petrous portion. The 'possible bone' in **Appendix III Plate 3.42** is also tentatively identified: it may be timber or metal.

C.102/10/12

This is the easternmost tank identified in Trench 1 in Feature 1 during Phase II. It was previously reported on in full (see McCullagh, 2016).

C.82/11

This is the westernmost tank identified in Trench 1 in Feature 1 during Phase II. It was previously reported on in full (see McCullagh, 2016).

C.84/85

This tank was immediately to the west of tank C.82/11. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.43** is a general annotated photograph of the base of the tank, while **Appendix III Plate 3.44-**

3.50 show the identified elements in more detail. Human skeletal remains were identified in the north (a), middle (b) and (d), and south (c) of the tank.

The identified human remains are summarised in **Table 3.7**.

Location as indicated in primary photograph Plate 3.43	Details	Plate reference (see Appendix III)
a	Multiple bones of at least one infant (<1 year), with evidence of articulation	3.44, 3.45, 3.46
b	Possible infant (<1 year) bones	3.47
c	Probable infant (<1 year) remains, with evidence of articulation	3.48, 3.49
d	Single possible fragment of human bone	3.50

Table 3.7: Identified human skeletal remains within tank C.84/85

Multiple, apparently primarily infant, skeletal remains were evident at the northern end of the tank, marked (a) in **Appendix III Plate 3.43**. These are highlighted in **Appendix III Plates 3.44-3.46**. The infant left temporal, indicated in **Appendix III Plate 3.44**, and highlighted in **Appendix III Plate 3.45**, is probably from an individual aged between 0-5 months at the time of death (after Humphrey and Scheuer 2006; referenced in Schaefer et al. 2009). A concentration of overlapping cranial bones, again probably from an infant, as well as long bones, was also visible in this northern area. At least two of the bones, **Appendix III Plate 3.46**, are suggestive of articulated forearm bones (radius and ulna).

A number of bones, possible from an infant/s, were also present along the western wall (see **Appendix III Plate 3.47**).

Numerous skeletal remains were present in the southern end of the tank and are detailed in **Appendix III Plates 3.48** and **3.49**. Certainly infant remains (<1 year) were present, although it is entirely possible that bones of young juvenile/s (1-6 years) are also present.

The ribs indicated in **Appendix III Plate 3.48**, may be articulated. In particular the ribs that overlie the cranial fragment and are also visible in **Appendix III Plate 3.49**, are aligned as if they were still at least partially articulated. A possible radius and ulna (bones of the forearm), which are visible in **Appendix III Plate 3.49**, also may be in an articulated state. In addition, the two parietals (left and right sides of the skull), indicated in **Appendix III Plate 3.49**, appear to represent a relatively intact cranium, particularly with the presence of a left petrous portion of the temporal (side of the skull).

A single fragment of bone was identified in the east (see **Appendix III Plate 3.50**).

C.86/87

This tank was immediately to the west of tank C.84/85. It comprised a single narrow chamber. No human skeletal remains were visibly within the extant deposits. **Appendix III Plate 3.51** is a general photograph of the surface of the tank sediments.

C.88/89

This tank was immediately to the west of tank C.86/87. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.52** is a general annotated photograph of the base of the tank, while **Appendix III Plates 3.53-3.60** show the identified elements in more detail. Human skeletal remains were identified throughout the length of the tank in at least five concentrations, running from (a) in the north end to (e) in the southern end.

The identified human remains are summarised in **Table 3.8**.

Location as indicated in primary photograph Plate 3.52	Details	Plate reference (see Appendix III)
a	Multiple bones of infants/young juvenile (<6 years)	3.53
b	Multiple bones of infants/young juvenile (<6 years)	3.54
c	Multiple bones of infants/young juvenile (<6 years)	3.55
d	Multiple bones of infants/young juvenile (< 6 years)	3.56
e	Multiple remains including loose cranium of a 1.5-2.5 year old and two possible infants (3 humeri)	3.57, 3.58, 3.59, 3.60

Table 3.8: Identified human skeletal remains within tank C.88/89

Juvenile human skeletal remains were visible throughout the length of this trench, as indicated in **Appendix III Plate 3.52**. Numerous fragments of infant and/or juvenile bones were present in the areas marked (a), (b), and (c), and also in (d), see **Appendix III Plates 3.53-3.56**. In the area (d), a possible humerus was identified from either an infant (<1 year) or a young juvenile (1-6 years), (see **Appendix III Plate 3.56**).

The southern end of the tank, indicated as (e) in **Appendix III Plate 3.52**, contain the most diagnostic fragments in tank C.88/89. Most notable, is the complete cranium (**Appendix III Plate 3.57**). The dental remains of this individual suggest that the mandibular second deciduous molars were just beginning to erupt at the time of death. This suggests an age of perhaps 1.5-2.5 years, although it would not be unexpected if the actual age-at-death was slightly older. The cranium is clearly disarticulated and is the only complete skull in all of Feature 1 which lies completely above the sediment of the tank. Other fragments were identifiable in this area. Three possibly infant (<1 year) possible humeri (upper bone of the arm) were identified in this area (**Appendix III Plates 3.59** and **3.60**), although only one could be identified as a possible right humerus (**Appendix III Plate 3.60**). This suggests the remains of two possible infants. The right thoracic/lumbar arch, visible in **Appendix III Plates 3.58** and **3.60**, had not fused to the left at the time of death, which suggests certainly an individual less than 2 years, and probably an individual less than 1 year (an infant). The arch appears small in comparison to the possible humeri, but this is not conclusive evidence of a third younger infant. A juvenile vertebral body was also identified in **Appendix III Plate 3.59**. The shape suggests an individual aged between 1-6 years at the time of death, that is, a young juvenile.

The right humerus in **Appendix III Plate 3.60**, is one of the few long bones which appears to show some, presumably post-mortem, erosion of the distal end (near the elbow).

C.90/91

This tank was immediately to the west of tank C.88/89. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.61** is a general annotated photograph of the base of the tank, while **Appendix III Plates 3.62-3.69** show the identified elements in more detail, with an additional feature indicated in **Appendix III Plate 3.70**. Human skeletal remains were identified near the middle of the tank (a), and in the southern half, (b) and (c).

The identified human remains are summarised in **Table 3.9**.

Location as indicated in primary photograph Plate 3.61	Details	Plate reference (see Appendix III)
a	Single young juvenile (1-6 years) cranial fragment	3.62
b	Probable infant (<1 year), with possible articulation	3.63, 3.64, 3.65
c	Infant/young juvenile (<6 years) remains of possibly two individuals, with possible articulation	3.66, 3.67, 3.68, 3.69

Table 3.9: Identified human skeletal remains within tank C.90/91

A fragment of a juvenile cranium was present on the western side of the tank (a), see **Appendix III Plates 3.61** and **3.62**. Two major concentrations of human bone were present in the southern half of the tank. The first (b), see **Appendix III Plates 3.63** and **3.64**, contained a probable/possible infant cranial bones, a set of infant right ribs, a right ilium (part of the right hip bone), infant arm bones, and a possible infant scapula.

When examined more closely (**Appendix III Plate 3.64**), a possible ischium (another part of the hip) was identified under the right ilium, and possible articulated vertebrae were also identified. These were adjacent to the set of right ribs and another set of possibly articulated bones that could not be identified. In addition, the aforementioned arm bones can also be seen in more detail in **Appendix III Plate 3.65**. In this case a right humerus, probably from an infant (<1 year) was identifiable, with an unsided radius and another long bone which may be an ulna. These are the bones that form the arm. The occurrence of these three bones together is unlikely to be coincidental and these arm bone may be approximately articulated. In fact, it is possible that the arm bones along with the set of right ribs, the possible scapula, the possible articulated vertebrae, and the pelvis bones are all approximately *in situ* as they would be in the approximate correct position for an infant lying on the left side.

Near the southwest corner of the tank, another dense concentration of skeletal remains was present (see **Appendix III Plates 3.66-3.69**). Identified bones included those of the cranium, ribs, a right scapula, and a possible ulna.

Three concentrations of apparently articulated ribs (**Appendix III Plate 3.67**) were apparent which suggests possibly two individuals. A right scapula was recovered adjacent to one set of right ribs (**Appendix III Plate 3.68**), which may suggest some degree of articulation.

Cranial remains were identified (**Appendix III Plate 3.69**), which may represent a relatively intact, but collapsed cranium of an infant or young juvenile (<6 years). The left frontal and temporal in particular are in the correct position for an articulated infant/juvenile cranium (see **Appendix VI B**), while a larger cranial fragment underlies the two: that larger fragment may be a parietal or the squama from the occipital.

Finally, the remains of a blue shoe from a young juvenile was present near the northern end of the tank (see **Appendix III Plates 3.61** and **3.70**).

C.92/93

This tank was immediately to the west of tank C.90/91. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.71** is a general annotated photograph of the base of the tank, while **Appendix III Plates 3.72-3.76** show the identified elements in more detail. Human skeletal remains were identified in the northern end (a), and in the southern half, (b), (c), (d), and (e), of the tank.

The identified human remains are summarised in **Table 3.10**.

Location as indicated in primary photograph Plate 3.71	Details	Plate reference (see Appendix III)
a	Young juvenile juvenile (2-6 years) cranium	3.72
b	Possible young juvenile (1-6 years) mandible	3.73
c	Multiple fragments including long bones of juveniles possibly aged *c.* 2 years (or slightly older)	3.74
d	Ribs and possible scapulae of young juvenile (1-6 years), possible articulation	3.75
e	Possible cranial vault, probable juvenile (<6 years)	3.76

Table 3.10: Identified human skeletal remains within tank C.92/93

Cranial remains are present in the northeast corner of the tank (**Appendix III Plate 3.72**). These may comprise a quite complete cranium, as at least the left parietal and left temporal (sides of skull) and the frontal bone (forehead) are present. The metopic suture appears fully closed. This typically fuses between the ages of 2-4 years (after Schaefer et al. 2009, 38).

Along the eastern wall of the tank there is a fragment of a cranium, and a mandible (**Appendix III Plate 3.73**). The mandibular symphysis is fused indicating an individual >1 year at the time of death (after Schaefer et al. 2009, 64). Indeed, the mandible actually appears quite robust and certainly indicates a juvenile at least aged between 1-6 years, but could be older. Unfortunately the teeth are unobservable. A possible hand phalanx was also identified but it was not possible to determine if there was any fusion of the proximal epiphysis (which would be expected in an adolescent individual).

Multiple bones were present just to the south of the central area of the tank (**Appendix III Plate 3.74**). A possible right tibia was present. The length of this was estimated based using the approximate estimated width (0.40m) of the tank near the base: the tibia was determined to be approximately 140mm in length, which suggests an age-at-death of approximately 2 years (after Maresh 1970). This was slightly unexpected as the tibia appears quite robust. However, the perspective at a depth of *circa* 2m is quite deceptive. The proximal end of a right femur (hip end of thigh bone) of a juvenile (1-6 years, age cannot be specifically determined although it may be similar in age to the aforementioned tibia) was identified overlying a cranial fragment. A vertebral body was also identified although unfortunately, it was not possible to assess the degree of fusion, if any, with the neural arch, which would help in determining the age-at-death.

A small collection of bones is visible in the southwest corner of the tank (**Appendix III Plate 3.75**). It was difficult to determine what bones are present. However, it is suggested that they are young juvenile (1-6 years) in origin and may comprise some left ribs and possibly the acromion of the scapula (shoulder blade), which may be suggestive of some degree of articulation. In the southeast corner, a possible cranial vault fragment was identified (**Appendix III Plate 3.76**).

C.94/95

This tank was immediately to the west of tank C.92/93. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.77** is a general annotated photograph of the base of the tank, while **Appendix III Plates 3.78-3.83** show the identified elements in more detail. Human skeletal remains were identified in the northern end, (a) and (b), and in the southern half, (c), (d), and (e), of the tank.

The identified human remains are summarised in **Table 3.11**.

Location as indicated in primary photograph Plate 3.77	Details	Plate reference (see Appendix III)
a	Probable infant (0-12 months) left femur	3.78
b	Cranium of young juvenile (1-6 years)	3.79
c	Concentration of bone, at least one juvenile, possibly aged 4-6 years	3.80, 3.81
d	Cranial remains of probable young juvenile (1-6 years)	3.82
e	Maxilla of young juvenile (1-6 years)	3.83

Table 3.11: Identified human skeletal remains within tank C.94/95

An infant left femur was identified in the northwest corner (**Appendix III Plate 3.78**), while a cranium, lying with the base facing upwards, was identified in the northeast corner (**Appendix III Plate 3.79**). The cranium is probably from a young juvenile (1-6 years).

A concentration of bones was apparent near the middle of the tank, (c) and (d), which mostly comprised disarticulated cranial fragments of at least one young juvenile (1-6 years), as well as a number of ribs, vertebrae, and at least one long bone. The ulna, identified in **Appendix III Plate 3.80** and **3.81**, is estimated to be approximately 140mm in length, which would suggest an age-at-death of approximately 4.5 years (after Maresh 1970). A body of a vertebral (actual vertebrae unidentified) appeared to be at least partially fused to the neural arch (which completes the bony channel for the spinal cord). These elements fuse at different times in different vertebrae: in the cervical (neck) vertebrae the body and neural arch are fused by 4 years, in the thoracic (which articulate with the ribs) vertebrae those elements fuse by 6 years, and in the lumbar (lower back) vertebrae the body and arch fuse by 5 years (after Schaefer et al. 2009, 120-121). There is certainly some fusion in the vertebrae observed in tank c.62, although it is not possible to confirm which vertebra it actually is. It does however, at least suggest the presence of an individual aged perhaps between 4-6 years at the time of death. A concentration of cranial bones lay nearby (see **Appendix III Plate 3.82**). Finally, the left maxilla of a probable young juvenile (1-6 years) was identified in the southeast corner of the tank (see **Appendix III Plate 3.83**). The rate of eruption and/or development of the teeth was not observable although it is probable that at least the first left upper deciduous molar had erupted.

C.96/97

This tank was immediately to the west of tank C.94/95. It comprised a single narrow chamber. Human remains were identified in the deposits. **Plate 3.84** is a general annotated photograph of the base of the tank, while **Appendix III Plates 3.85-3.87** show the identified elements in more detail. Human skeletal remains were identified at the northern (a) and southern ends (b) of the tank.

The identified human remains are summarised in **Table 3.12**.

Location as indicated in primary photograph Plate 3.84	Details	Plate reference (see Appendix III)
a	Cranial bones, ribs, possible scapula of at least one infant/young juvenile, some possible articulation	3.85
b	Infant (0-12 months) remains including possible an articulated cranium and cervical vertebrae	3.86, 3.87

Table 3.12: Identified human skeletal remains within tank C.96/97

At least two separate cranial bone fragments were visible at the northern end of the tank (see **Appendix III Plate 3.85**). In addition, there appeared to be a set of ribs (medial ends) overlying a possible scapula (lateral border), which may suggest some degree of articulation. It is difficult to determine the age at death but the remains would certainly appears to be either infant (<1 year) and/or young juvenile (1-6 years).

A number of infant bones were identified in the southern end of the tank (**Appendix III Plate 3.86**). Cranial remains are clearly visible in two locations, as well as numerous rib and vertebral bones, and a left tibia. The main concentration of cranial bones (see **Appendix III Plate 3.87**), comprised a left and a right parietal (sides of the skull) and an occipital (back of the skull), as well as some possible cervical (neck) vertebra. This suggests that these elements may be largely intact and may retain some degree of articulation (see **Appendix VI B**).

C.98/99

This tank was immediately to the west of tank C.96/97. It comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.88** is a general annotated photograph of the base of the tank, while **Appendix III Plate 3.89-3.91** show the identified elements in more detail. Human skeletal remains were identified at the northern end of the tank (a), near the centre underneath a fallen slab (b), and in the southern half (c).

The identified human remains are summarised in **Table 3.15**.

Location as indicated in primary photograph Plate 3.88	Details	Plate reference (see Appendix III)
a	Possible infant (<1 year) cranial fragments.	3.89
b	Possible young juvenile (1-6 years) possible vertebral body	3.90
c	Possible young juvenile (1-6 years) cranial fragment	3.91

Table 3.13: Identified human skeletal remains within tank C.98/99

Possible infant cranial bones are present at the northern end of the tank (**Appendix III Plate 3.89**). A possible young juvenile (1-6 years) possible vertebral body was identified under a fallen slab near the east wall (**Appendix III Plate 3.90**), while a possible juvenile (<6 years) cranial fragment is present in the southern half (**Plate 91**).

C.100/101

This tank was immediately to the west of tank C.98/99 and to the east of tank C.104/105: the latter was identified in Trench 4 of the first phase of archaeological investigations. Tank C.100/101 comprised a single narrow chamber. Human remains were identified in the deposits. **Appendix III Plate 3.92** is a general annotated photograph of the base of the tank, while **Appendix III Plates 3.93-3.94** show the identified elements in more detail.

The identified human remains are summarised in **Table 3.14**.

Location as indicated in primary photograph Plate 3.92	Details	Plate reference (see Appendix III)
a	Young juvenile (1-6 years) cranial fragments	3.93, 3.94

Table 3.14: Identified human skeletal remains within tank C.100/101

A probable young juvenile (1-6 years) cranial, comprising at least two individual bones, was identified underlying the large fallen slab in tank C.100/101 (see **Plates 3.93-3.94**).

3. 4 Discussion

In total, 16 tanks were identified, opened, and recorded during the most recent phase (Phase IIA) of archaeological investigations at the former Bons Secour Mother and Baby Home in Tuam, Co. Galway. These 16 tanks, along with four identified and examined in 2016 (Phase II), were contained within a long concrete structure, built into the southern wall of the large cess pit associated with the Poor Law Union Workhouse which originally occupied the grounds. Human skeletal remains had been identified in all four tanks examined in 2016 , and human bone was also recovered, in a disarticulated state in deposits to the north of the north wall of the concrete structure. Samples of human bone taken from inside the tanks returned radiocarbon dates ascribed to the twentieth century. All identified human skeletal remains from 2016 were juvenile (<18 years) in origin, and specifically were from infants (<1 year) or young juveniles (1-6 years) (see McCullagh 2016).

No skeletal remains were physically removed during the Phase IIA investigation, and all osteoarchaeological analysis in this phase is based exclusively on the assessment of photographs taken of the 16 tanks. Human skeletal remains were identified in 14 out of the 16 tanks: the exceptions were tank C.62/63 and tank C.86/87. It should not be assumed however, that there are *no* human skeletal remains in those two tanks: the presence of human remains was only confirmed in tank C.100/101 when the camera was able to photograph underneath a fallen slab of concrete. It is probable, given that it is now known that there are human remains in at least 18 of the total of 20 tanks in Feature 1, that there are in fact human remains in tanks C.62/63 and tank C.86/87, but that they are simply not immediately visible on the surface.

It is impossible, given the limitations of the present archaeological investigation, to estimate the numbers of individuals represented in the tanks. It is clear however, that many tanks contain a mixture of infant (<1 years) and young juvenile (1-6 years) bones. For example, tank C.84/85 contained a large concentration of bones in the southern end of the tank where both infant (<1 year) and young juvenile (1-6 years) remains were identified. Only actual physical investigation could reveal the numbers of individuals deposited in Feature 1.

A cranium was present in tank C.88/89, possibly from an individual aged between 1.5 and 2.5 years, although it is possible that the individual was slightly older. This skull was unique in terms of complete crania in that it was sitting on the surface of the sediments. Also all other cranial fragments were at least partially embedded in the sediments, while tank C.50/51 (examined in 2016) contained a partially embedded cranium which may represent a relatively intact skeleton (McCullagh 2016). In contrast, the cranium in tank C.88/89 clearly lay on the surface of the sediments. This may suggest that the latter cranium was perhaps thrown into the tank in more recent decades and may even have originated from another location. It was interesting that, adjacent to the cranium, is an infant humerus which shows post-mortem erosion: this was quite unique in terms of the observed general preservation of other skeletal remains in the tanks as the bones were invariably in an excellent state of preservation. Again, it is possible that this long bone originated elsewhere (where it may have suffered the post-mortem erosion) and was subsequently redeposited within tank C.88/89.

In contrast to the aforementioned cranium and humerus in tank C.88/89, there were numerous examples of bones which appeared to be in at least some form of articulation, though not necessarily *in situ*. Possible articulated skeletal remains were identified in tanks C.52/53, C.54/55, C.56/57, C.58/59, C.84/85, C.90, C.92/93, and C.96/97. Most of these comprised sets of ribs, which appeared to have collapsed on top of each other, as would be normal in a decomposing body: up to four sets of ribs ('set' referring to a set of left ribs or a set of right ribs) were identified in tank C.90/91. In a number of cases, the bones of the forearm (radius and ulna) were tentatively identified lying together, suggesting some degree of articulation, such as in in tank C.58/59 and tank C.84/85. In tank C.90/91, numerous bones were suggestive of an infant lying on its left side.

The 'articulation' is not as clear as it would be in remains that had actually been buried. The nature of the tanks has dictated the current state of the skeletal remains. As was surmised in the original osteoarchaeological assessment (McCullagh 2016), it is probable that complete bodies were deposited in the tanks: this would at least explain the excellent state of preservation of the observable bone. If the bones had been dug up elsewhere and then redeposited in the tanks, it would be expected to see much more fragmentation and it would be unlikely that there would be relatively intact juvenile crania, such as in tank C.92/93 (see **Appendix III Plate 3.72**) and tank C.96/97 (see **Appendix III Plate 3.87**). In addition, it would be expected that the redeposited earth would be visible in the tanks. Instead however, all visible sediments in the tanks may in fact be formed as part of normal fluctuations within and into the tanks.

It is probable that there was some fluctuation in terms of water levels within the tanks. It was evident in most tanks, that the sediments (now quite dry), had shrunk back from the edges of the tanks. This would suggest that, at one stage, the interiors of the tanks may have been substantially wetter. Assuming that complete bodies were deposited in the tanks (with no actual burial in the sense of covering the remains with earth), then fluctuations in the water table would have allowed bodies, and later body parts and bones, to float and disperse across each tank. In forensic contexts it is known that 'dangling appendages' will separate from the main carcass, and the water action will allow for additional dispersal (Haglund and Sorg 2002). Interestingly, a lot of the bone concentrations were on the south sides of the tanks: this would represent the normal drainage of the site where the higher ground was to the north. The assumed fluctuations in water levels would certainly account for the somewhat unusual manifestations of 'articulation', for example where sets of ribs in particular were commonly identified. Interestingly, in some tanks skeletal remains were identified which were not within the sediments. In tank C.54/55 two possible fragments of bone were noted on the north facing wall of the tank (**Appendix III Plate 3.14**), although the identification was quite tenuous. However, more conclusively, in tank C.58/59 a single infant/young juvenile probable hand phalanx was recorded attached to the south-facing wall of the tank (**Appendix III Plate 3.32**). The hand phalanx in particular was located well above the current sediment level, suggesting that there was indeed fluctuation in the water table within the tanks.

The age-at-death span of the skeletal remains examined in 2016 was from 35 foetal weeks to 2-3 years (McCullagh 2016). No skeletal remains were recovered during the most recent investigation. However, the osteoarchaeological assessment of the photographs suggests a similar age range for the individuals identified in the newly examined tanks: all of the skeletal remains were probably from individuals aged less than 6 years at the time of death (that is, infants <1 years and young juveniles aged 1-6 years). In reality, most were probably in the younger end of that scale. However, there was an exception. In tank C.94/95 a vertebra and an ulna were identified that are probably from an individual aged between 4-6 years at the time of death.

Finally, again referring to the deposition of the remains, one piece of timber had an unusual angle in tank C.60/61 (see **Appendix III Plates 3.37** and **3.38**). This was reminiscent of the angles which may be seen in a coffin and the timber does not appear as crude as most of the shuttering from the construction of the tanks which had collapsed in. However, the identification of this 'coffin' is tenuous and should not be taken as conclusive. The possible wickerwork identified in tank C.54/55 (see **Appendix III Plate 3.15**) may be related to the deposition of a body or bodies but again the identification is not definite. It is unknown if the black plastic comb in tank C.58/59 (see **Appendix III Plate 3.33**) and the blue shoe in tank C.90/91 (see **Appendix III Plate 3.70**) are contemporary with the deposition of human remains.

4. Artefactual Evidence

This excavation was intended to be non-intrusive exercise and solely for the purposes of establishing the extent of Feature 1 and provide an indication of the extent of the deposition of human remains contained therein. Excavation was not possible due to limited accessibility and resulting safety issues, thus artefact recovery did not take place. There was a single exception to this.

It was observed that a piece of evidence in the form of a plastic bottle lay directly on the surface of C. 95 within chambered tank C. 94. There was ongoing consultation and agreement with the MBHCOI throughout the work, and it was acknowledged at the time that it was pertinent to recover this as an exhibit, as it could be done so without causing disturbance to the deposit (C.95) and human remains therein. The context could be considered secure and thus the bottle of significant evidential value.

This bottle may be described as a moulded green plastic bottle with the label 'Castrol GTX' printed directly onto the plastic, it was empty of contents. The text on the label reads in full "Castrol GTX HIGH PERFORMANCE MOTOR OIL", "CONTENTS 500ml" and "CASTROL (IRELAND) LIMITED". There is no evidence remaining of a serial number or other individual identifying features. The bottle was in an excellent state of preservation despite being slightly crushed on one side. The green plastic had degraded slightly with a gold foil cover remaining over the bottle opening. There was no evidence of the original bottle cap, see **Appendix III Plates 4.1 and 4.2.**

Subsequent enquiries with the manufacturer revealed that this product was released into the UK market on the 18th April 1968. This particular product did not exist prior to this date. It would have been available in the Irish market on or after this date but not before**, see Appendix III Plate 4.3. '***This product used the same technology of 'liquid tungsten' as the new formula Castrol, it was an instant success and has become one of the longest lasting of the Castrol brands'* (Information supplied by Joanne Burman of the BP Archive, BP International, Coventry, United Kingdom).

These findings indicate that these chambered tanks were accessible, either temporarily or for an extended period of time, post 1968. When combined with the radiocarbon dating of Phase II (1925-1957) and based on the history of the site-use, this evidence makes it highly likely that the chambered tanks were accessed at, or during, the time of the construction of the Tuam Road Housing Estate. Other debris within the chambered tanks support the suggestion that there is, what can be considered non-domestic, waste disposed in these tanks subsequent to the deposition of the human remains, e.g. contents of C.11/82 see **Appendix IV Figure 4.1.**

5. Environmental Sampling results

Soil samples were submitted to Dr Lorna DAWSON at the James Hutton Institute, Scotland. Samples were subjected to Volatile Organic Compound (VOC) analysis, organic analysis and isotope analysis. VOC analysis was conducted on an initial 32 soil samples submitted to Lorna DAWSON. This was followed by and independent alkane/sterol/alcohol analysis on 11 of what were considered the most 'interesting' of the samples. These samples were selected based on the initial screening, the results of which are described in full in **Appendix VII**.

5.1 Examination

Soil is a mixture of both inorganic and organic material (Dawson and Hiller, 2010; Dawson and Mayes, 2014). The Organic material reflects the plant and animal material having been deposited or decomposed within that soil and also human organic inputs to the soil (Dawson and Mayes, 2014). A combination of gas chromatography and gas-chromatography spectrometry (GCMS) can be used to characterise and identify many organic compounds in oils, both volatile and physical which helps ascertain what those inputs likely were.

Comparison of the distribution of the volatile compounds found in the samples with published data describing the range of volatile compounds found in the samples with published data describing the range of volatile compounds produced during decomposition of mammalian tissues, including humans (Vass et al., 2004, 2008; Vaas, 2012) allows the interpretation of contact with human decomposition products to be made. This use of the odour of decomposition is relatively recent and is considered an experimental technique for intelligence and is still under development (Dawson, Sheperd and Mayes, **Appendix VII)**.

5. 2 Summary of Findings

The examination confirms that there is evidence that this site had previously been used as a sewage treatment facility. The result of these tests cannot categorically establish if the sewage treatment facility was in use contemporaneous with the deposition of human remains.

These tests also cannot contribute to the hypothesis of whether the human remains had decomposed prior to being deposited in the tanks or if they were deposited and decomposed *in situ*. A number of compounds indicative of bone decomposition, ketones, aliphatic alcohols and *n*-aldehydes, were found in locations with high bone density.

Some of the results from soil sample analysis indicate the presence of faecal material but it is also likely that the human remains have contributed to these indications. There were markers of human sewage in the chambered tanks as well as human decomposition products. Dr DAWSON found that it was difficult to say categorically if the chambered tanks were in use at the time the bodies were deposited there.

The samples were found to have very low concentrations of biomarkers that would typically indicate sewage. Dr DAWSON found that the reasons for low biomarker concentrations found in samples are not easy to assess. If the chambers represented a closed cesspit or sewage treatment facility it is possible that the collected sewage had been removed before the deposition of the human remains. Soil may have been added at the time of deposition or soil may have seeped in from the roofs or openings at the base. If there were one or more pipe outflows (i.e. the facility was a septic tank, or was connected to a sewer outflow), it is expected that little sewage would be left behind. These low values could be as a result of several actions; old sewage, partial removal of sewage or the mixing of other inert material such as soil from elsewhere.

6. Conclusion

6.1. Condition of Site Post Excavation

Following the completion of the investigations of Feature 1, a series of stages of covering layers, both permeable and impermeable, were placed over the concrete tank to protect the chambered tanks from intrusion and to ensure that the site was secure in terms of safety and preservation. These measures are not intended for permanency.

The entire length of the top of the concrete tank (C.5) was first covered with heavy gauge plastic, this was followed by custom designed steel sheets. This was followed by further heavy gauge plastic, to delay oxidation/corrosion, followed by a layer of topsoil, over which a permeable breathable membrane was laid. Finally, a layer of gravel was spread over all of the aforementioned covering layers. The site was levelled and left in a tidy condition prior to departure (see **Appendix III Plates 6.1 and 6.4**).

All reasonable measures were put in place to secure the site temporarily, with a consideration of a <6-month time frame. The hoarding surrounding the site is also a temporary measure that has been in place since September 2016 and may significantly deteriorate within a short timeframe. The gate through the hoarding was fixed with a lock and a copy of the key to the lock was passed to An Garda Síochána, Tuam. The MBHCOI is also in possession of a key. This lock can be 'cut' at any time and should not be considered prohibitive nor a long-term solution.

6.2 Conclusion

The full extent of the chambered structure was investigated from the near-surface during this phase. The complex nature of the site limited the extent of investigative work to observation and full recording, in conjunction with a soil sampling programme conducted in the latter half of site work.

The structure itself, Feature 1, is a later addition to the 19th century workhouse 'sewage tank' that appears on the 1892 edition of the Ordnance Survey mapping (McCullagh, 2016). It has been constructed on the internal face of the south wall of the stone and mortar 'sewage tank', and it may be considered a possible upgrade to the pre-existing sewage treatment facility. The walls are constructed of stone and shuttered concrete. Each of the twenty chambers has been constructed with shuttered concrete with the easternmost chambers having openings at their base, 2.75m below current ground surface. Structural evidence suggests it is possibly an unfinished or abandoned structure as discussed in Section 2. The exact date of construction of Feature 1 is unclear. However, radiocarbon dating and archaeological evidence from Phase II indicates construction would have taken place pre 1940.

As described in section 3, 18 of the 20 chambers in Feature 1 contained observable juvenile human remains; the two remaining chambered tanks would require further investigation. Osteological analysis considers the observable human remains here to be excellently preserved. Articulation at the time of deposition is considered probable. It was not possible to determine through soil analysis if the facility was in use for sewage treatment during the time of the deposition of human remains.

The results of this investigation highlight further the extent of juvenile human remains that are deposited at this location. This is not a recognised formal burial situation. The structural evidence here implies that a sewage treatment facility was reused for the interment of juvenile human remains.

Acknowledgements

The authors of this report would like to acknowledge the invaluable co-operation of An Garda Síochána, Tuam, Galway County Coroner, and the Office of the State Pathologist for their assistance on site during excavations.

7. Qualifications and Experience of Contributors

Niamh McCULLAGH BA MA MSc MCSFS

Forensic Archaeologist, Project Director Phase IIA

Niamh is an independent consultant Forensic Archaeologist specialising in the search, location and recovery of human remains in a forensic context. As a Forensic Archaeologist, Niamh has worked nationally and internationally on both current and historic casework and she also provides input to training capacity for Forensic Archaeologists. Niamh is Senior Forensic Archaeologist to the Independent Commission for the Location of Victims Remains and has assisted An Garda Síochána in the investigation of multiple criminal cases. She has a BA Major in Archaeology (University College Cork, 2001), MA Archaeology (University College Cork, 2002) and MSc Forensic Archaeology and Crime Scene Investigation (Bradford University, 2007) and has published a number of papers in relation to her specialism. She is recognised as Professional Member of the Chartered Society of Forensic Sciences, an Expert Witness in Ireland, a member of the Irish Association of Forensic Practitioners and has represented Forensic Archaeology at a European level.

Aidan HARTE, BA MA MIAI

Senior Archaeologist and GIS Specialist

Aidan is an independent, qualified Archaeologist and Geographer, with over 15 years' archaeological experience in Ireland, the UK and France. He is a license eligible Archaeological Excavation Director as recognised by the Department of Arts, Heritage, Regional, Rural and Gaeltacht Affairs. He also continues to work as a Senior Team member with the Independent Commission for the Location of Victims Remains. He has been a full member of the Institute of Archaeologists of Ireland since 2007, has served on the Board of Directors for the Cork Historical and Archaeological Society since 2013 and has more recently been recognised as an Affiliate Member of the Chartered Society of Forensic Sciences. Aidan has lead excavations and surveys of over 35 archaeological sites, of various type, size and period, in a variety of locations and conditions. Following his primary degree, his master's degree in 'Methods and Practices in Irish Archaeology' (UCC) specialized in the use of GPS/GIS for which he was awarded the 'Past Perceptions Prize' 2002. With a diverse range of research interests, he has published papers on survey methodology, GIS and multiple archaeological site types.

Linda LYNCH. MA PhD MIAI

Human Osteoarchaeologist

Linda is a professional archaeological consultant and human osteoarchaeologist with over 20 years' experience in Irish archaeology. A member of the Institute of Archaeologists of Ireland, she also served on the Board for three years. She is a license-eligible archaeological excavation expert and a leading professional in the field of osteoarchaeology in Ireland, with a significant profile of publication and lecturing. She has particular expertise in issues similar to those encountered at the Children's Burial Ground at Tuam. Her Master's degree in 1998 focused on neonate and infant remains from *cillíní* or 'children's burial grounds'. In 2014 Linda was awarded a PhD in research that focused on human remains from 19th century workhouse burials. Linda was also the specialist employed to examine the skeletal remains recovered from the archaeological excavation adjacent to Tuam Poor Law Union Workhouse.

8. Appendices

Appendix I: Warrant issued

Mother and Baby Homes Commission of Investigation

Commissions of Investigation Act 2004

Sections 8, 26 and 28

WARRANT

TAKE NOTICE THAT in accordance with Section 26 of the Commissions of Investigation Act 2004 (hereinafter 'the Act')

Niamh McCullough

Of Cork in the County of Cork

Is a person appointed under Section 8 of the Act and is hereby Authorised to exercise the powers given under section 28 of the Act in relation to the premises known as the Children's Burial Ground located in the Dublin Road Housing Estate, Tuam, Co Galway.

Dated this 1st day of September 2016

JUDGE YVONNE MURPHY
CHAIRPERSON OF THE COMMISSION

Appendix II: Technical Note

The archaeological theories and techniques used during this search and excavation were in accordance with those outlined in publications such as:

1) 'Standards and Guidance for Forensic Archaeologists' (Powers and Sibun, 2011) prepared for the Chartered Institute for Archaeologists, UK.

2) Component Standards for Archaeology and Anthropology issued by the Chartered Society for Forensic Sciences, UK (www.forensic-science-society.org.uk).

3) Handbook of Forensic Anthropology and Archaeology (World Archaeological Congress Research, 2011), Blau, S. & Ubelaker, D. (eds).

4) 'Management of Archaeological Projects' (MAP2), produced by English Heritage (Andrews 1991).

5) Technical papers issued by the Institute for Archaeologists of Ireland (www.iai.ie).

6) Museum of London Archaeological Service Archaeological Site Manual (MoLAS, 1994).

Appendix III: Plates

Plate 1.1: Protection offered by commercial marquee.

Plate 2.1: Openings within C.5 looking west

Plate 2.2: Openings within C.5 looking east

Plate 2.3: Timber formwork *in situ* at C.46/47/62/63

Plate 2.4: Concrete lid consistent with original concrete structure

Plate 2.5: Repairs an replacements to lids

Plate 2.6: Evidence of damage to original lids.

Plate 2.7: Timber *in situ* for cast concrete cap (C.5) at C.73/74/92/93

Plate 3.1: C.52/53, annotated photograph of sections of identified human remains, see Plates 3.2-3.7

Plate 3.2: C.52/53(a), detail of infant cranial bones, see Plate 3.1

[redacted]

Plate 3.3: C.52/53(b), multiple infant bones at east end of tank, see Plate 3.1

Plate 3.4: C.52/53(c), infant cranium and long bone, see Plate 3.1

Plate 3.5: C.52/53(d), concentration of skeletal remains from multiple individuals, see Plate 3.1

Plate 3.6: C.52/53(d), detail, infant mandible, located at bottom edge of Plate 3.5

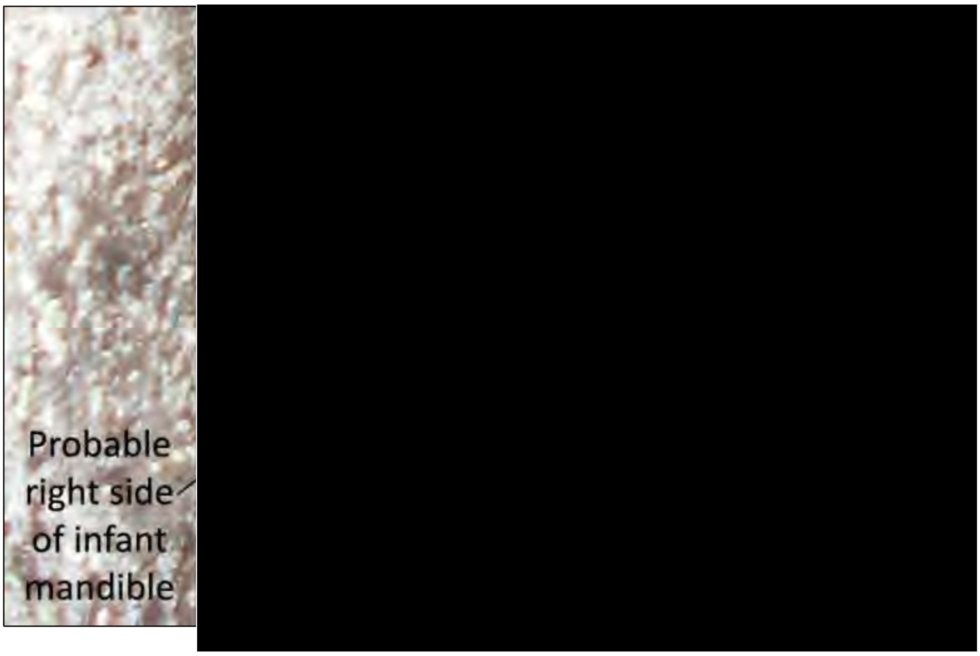


Plate 3.7: C.52/53(d), detail, infant mandible, north to bottom, located at right side of Plate 3.5

Plate 3.8: C.54/55, areas with identified human remains, see Plates 3.9-3.15

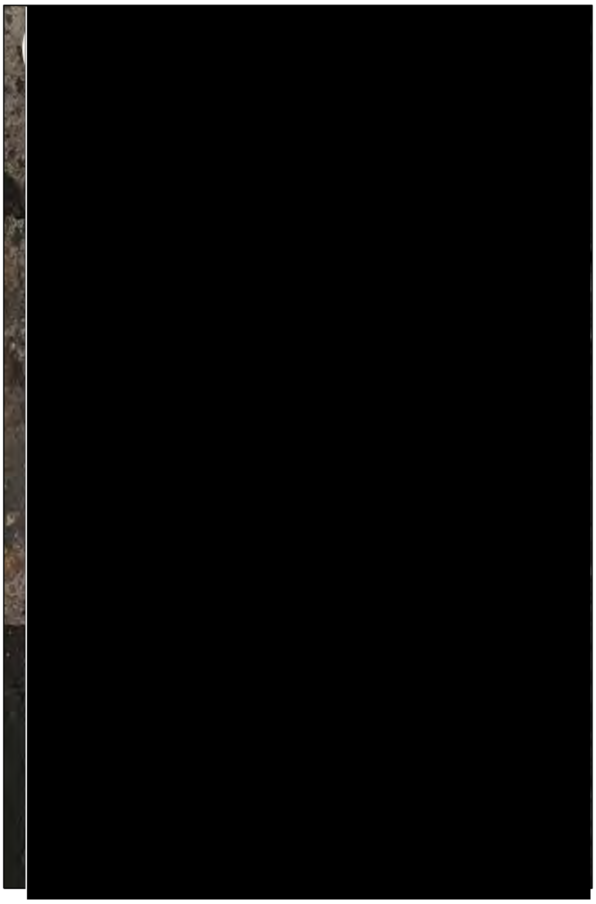


Plate 3.9: C.54/55(a), detail of infant/young juvenile bones (the petrous portion is part of the temporal bone of the cranium which houses the components of the ear), see Plate 3.8

Plate 3.10: C.54/55(a), detail of possible infant petrous portion (the petrous portion is part of the temporal bone of the cranium which houses the components of the ear) in area (a), see Plate 3.8


[redacted]

Plate 3.11: C.54/55(b), infant bones near south end of tank, see Plate 3.8

[redacted]

Plate 3.12: C.54/55(b), detail of infant femur and hand bones, possible indication of articulation, identified at western edge of tank, see Plates 3.8 & 3.11

Plate 3.13: C.54/55(b), detail of infant/juvenile cranial fragments with animal bone, identified at south end of tank, see Plates 3.8 & 3.11, north to bottom

Plate 3.14: C.54/55, north-facing wall of tank showing location of two fragments of possible human bone

Plate 3.15. Possible wickerwork located at northern end of tank C.54/55, see Plate 3.8

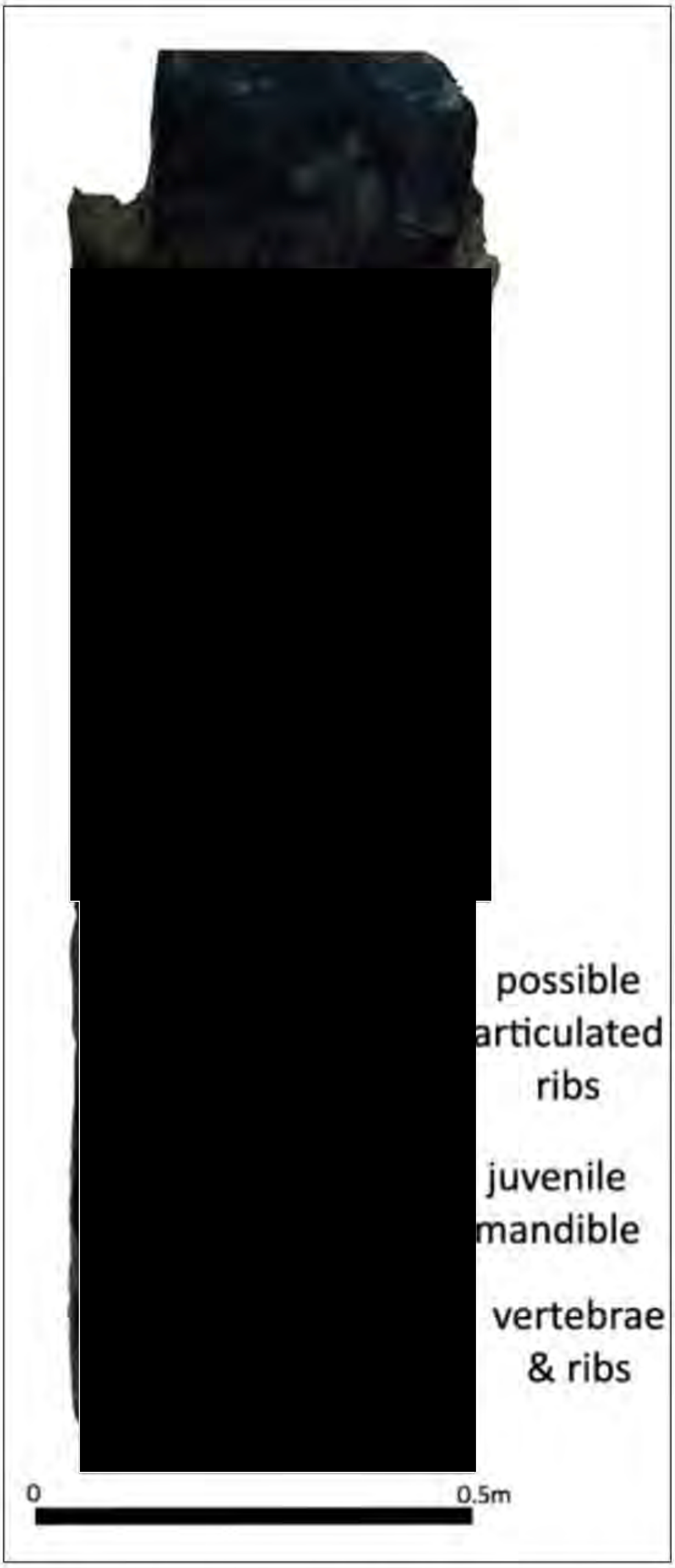


Plate 3.16: C.56/57, locations of identified human remains, see Plates 3.17-3.23

Plate 3.17: C.56/57(a), multiple infant/juvenile cranial bones at north end of tank, see Plate 3.16

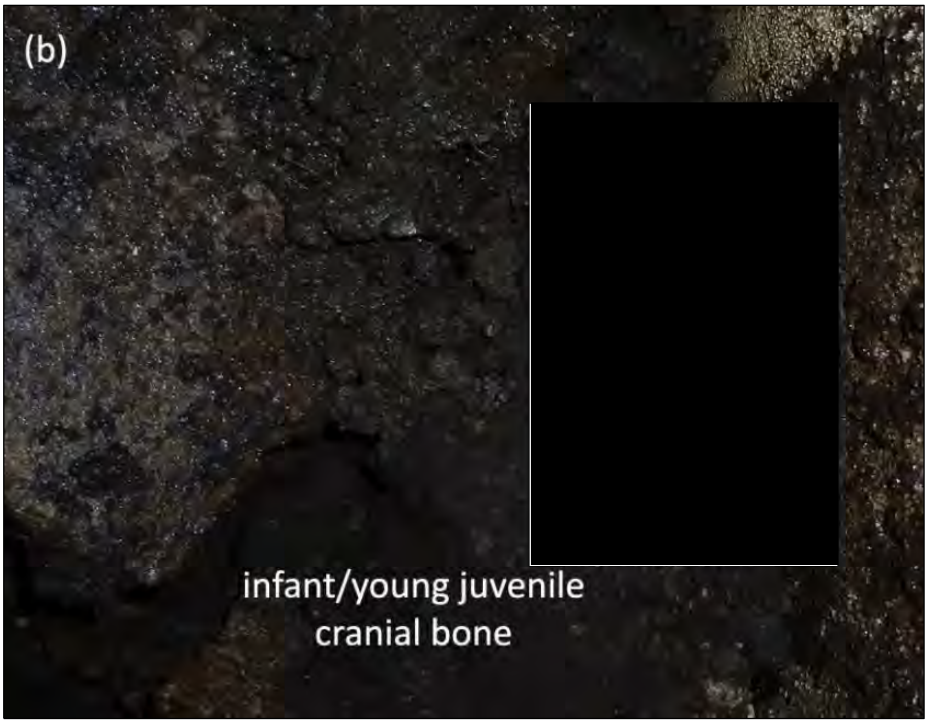


Plate 3.18: C.56/57(b), infant/juvenile cranial bone, identified on east side of tank, see Plate 3.16

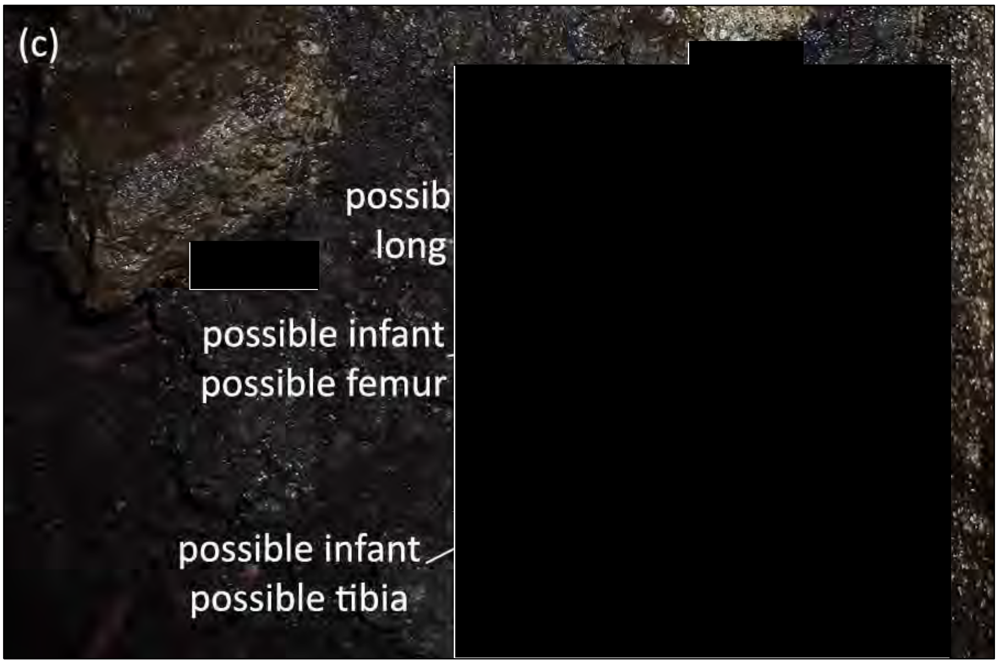
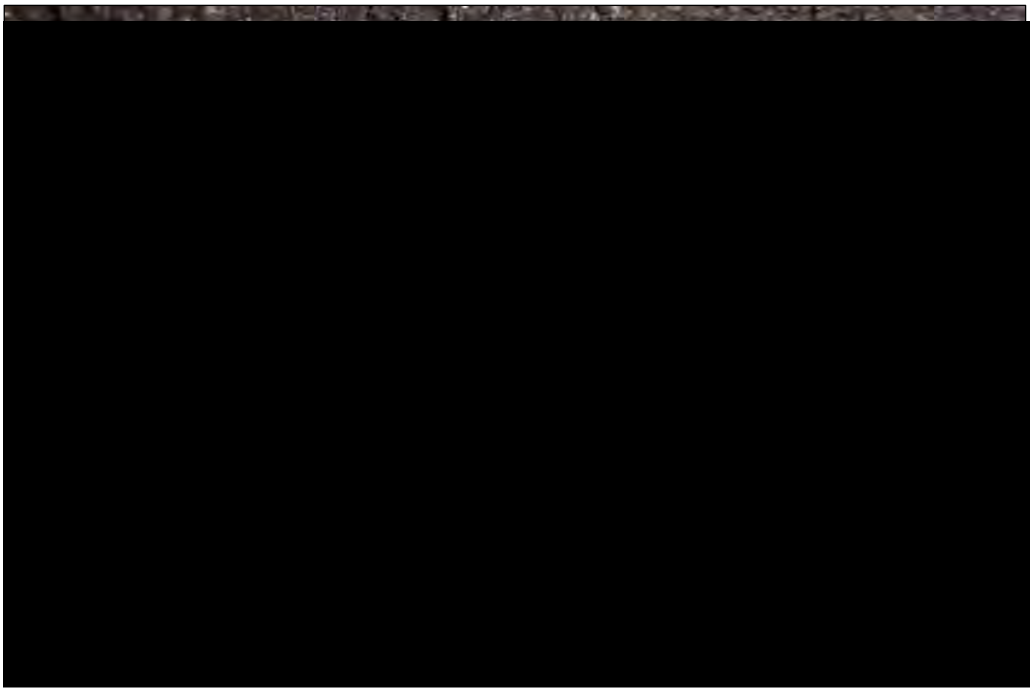


Plate 3.19: C.56/57(c), multiple infant remains, identified near middle of tank, see Plate 3.16

Plate 3.20: C.56/57(d), concentration of primarily young juvenile skeletal remains at southern end of c.56/57, see Plate 3.16

[redacted]

Plate 3.21: C.56/57(d), detail, possible articulated ribs, location indicated in Plate 3.16



[redacted]

Plate 3.22: C.56/57(d), detail, juvenile mandible (2-4 years) and young juvenile vertebral arch, location indicated in Plate 3.16

Plate 3.23: C.56/57(d), detail, collection of infant/young juvenile vertebral fragments and ribs, suggesting possible articulation, location indicated in Plate 3.16

Plate 3.24: C.58/59, annotated photograph of sections of identified human remains, see Plates 3.25-3.32, with additional feature in Plate 3.33

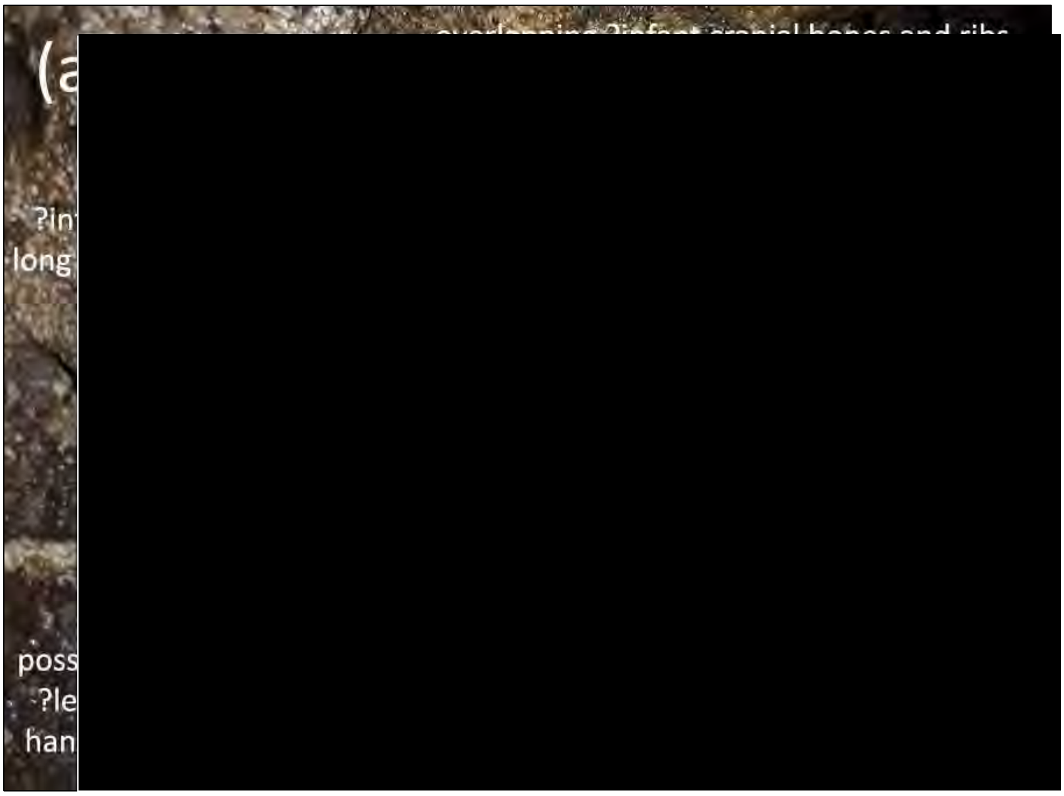

[redacted]

Plate 3.25: C.58/59 (a), multiple infant remains identified at northern end of tank, see Plate 3.24


[redacted]

Plate 3.26: C.58/59 (a) detail, detail of possible infant left ilium, indicated near top right of Plate 3.25

Plate 3.27. C.58/59(a) detail, detail of possible infant ulna and radius, indicated near centre of Plate 3.25

Plate 3.28: C.58/59(b), possible infant/young juvenile remains, see Plate 3.24, detailed in Plates 3.29-3.30

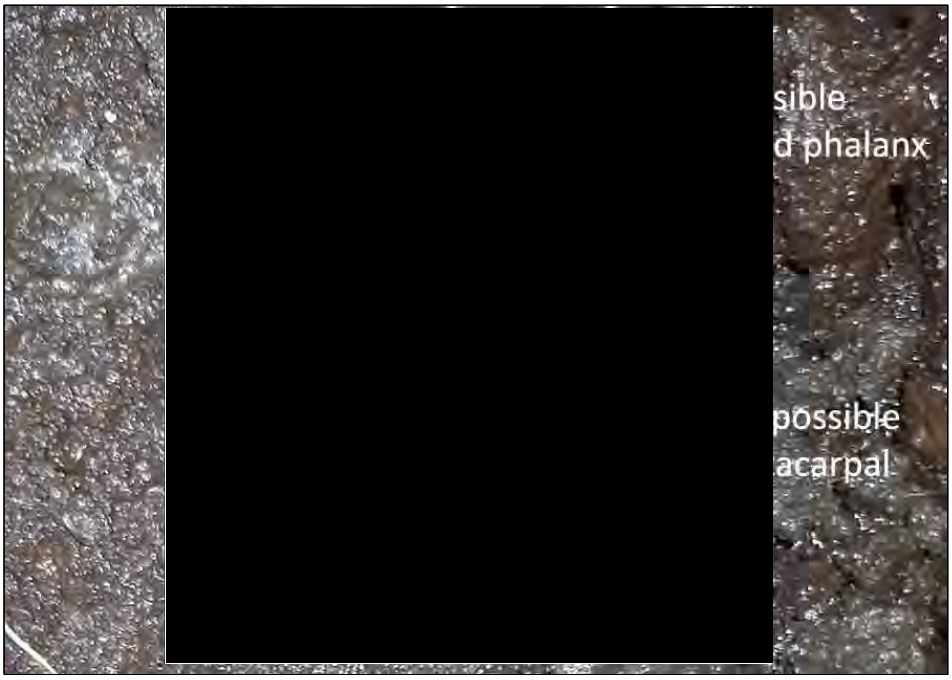


Plate 3.29: C.58/59(b) detail, possible infant hand bones, indicated in top half of Plate 3.28

Plate 3.30: C.58/59(b), detail, possible articulated infant/young juvenile left ribs and vertebrae, indicated in bottom half of Plate 3.28

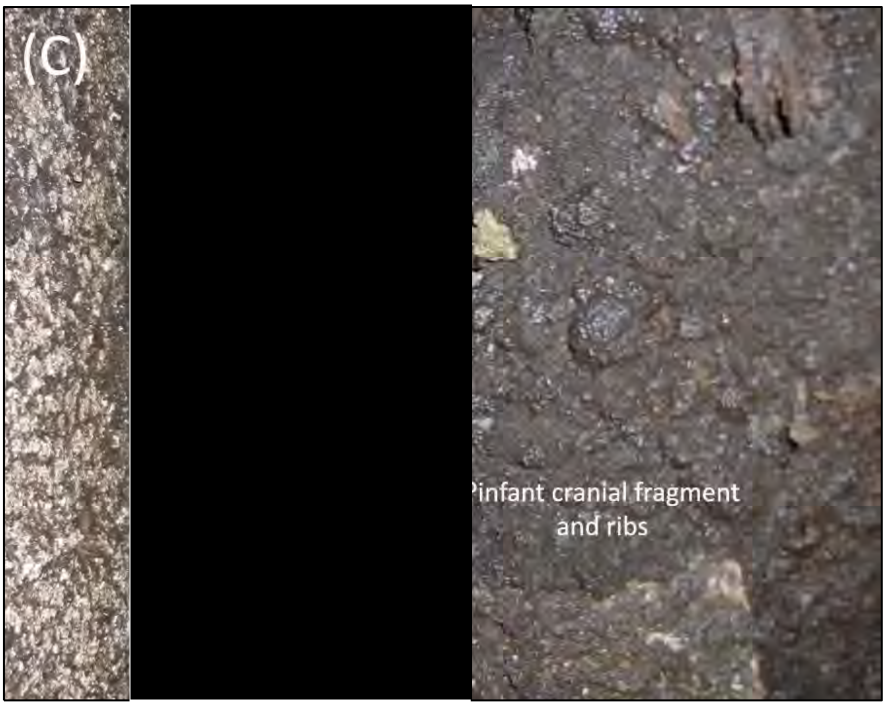


Plate 3.31. C.58/59(c), possible infant remains, see Plate 3.24

Plate 3.32: C.58/59, possible infant/young juvenile hand phalanx attached to wall in northwest corner

Plate 3.33: C.58/59, black plastic comb, see Plate 3.25 for location

Plate 3.34: C.60/61, annotated photograph of sections of identified human remains, see Plates 3.35-3.38

Plate 3.35: C.60/61(a), detail of infant and juvenile bones, see Plate 3.34

Plate 3.36: C.60/61(a), detail, possible infant bones, location indicated by arrow in Plate 3.34

Plate 3.37: C.60/61(b), detail of infant bones, see Plate 3.34

Plate 3.38: C.60/61, unusual edge evident in timber near southern end of tank (north to bottom, detail of inversion of Plate 3.37), which may be the possible edge of a coffin

Plate 3.39: C.62/63, no human skeletal remains identified

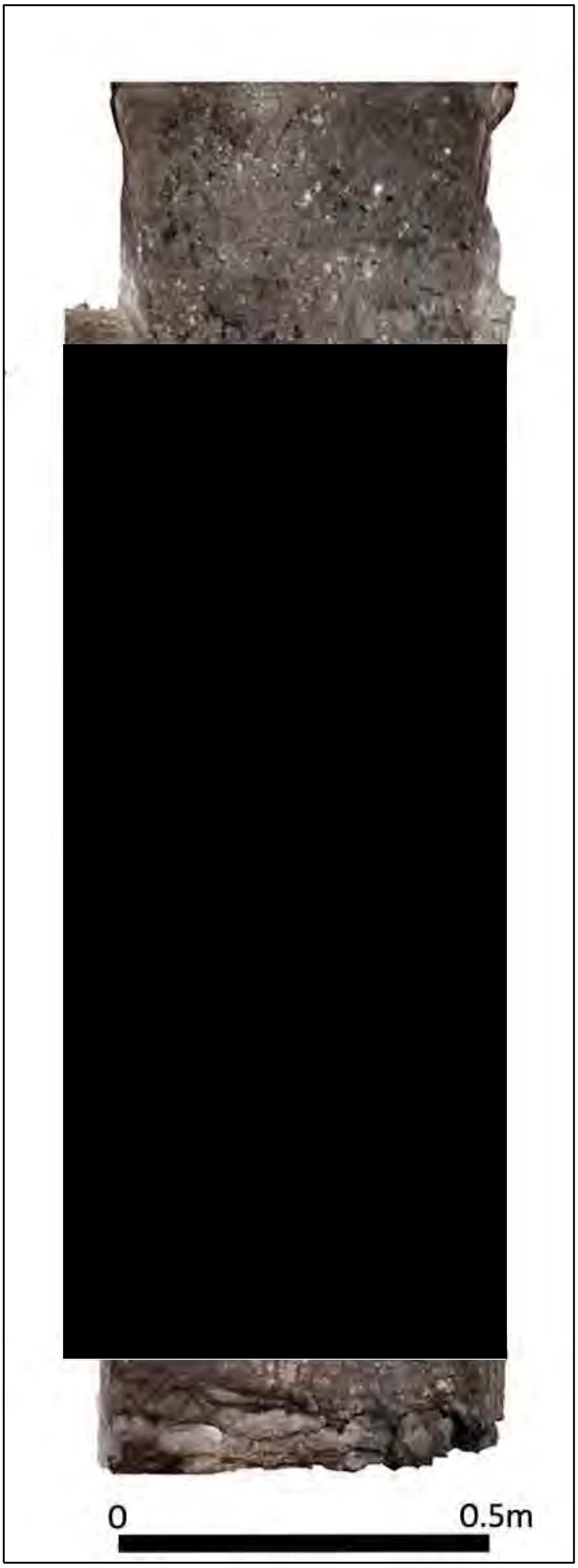


Plate 3.40: C.64/65, annotated photograph of sections with identified human remains, see Plates 3.41-3.42

Plate 3.41: C.64/65(a), detail of infant cranial fragments, see Plate 3.40

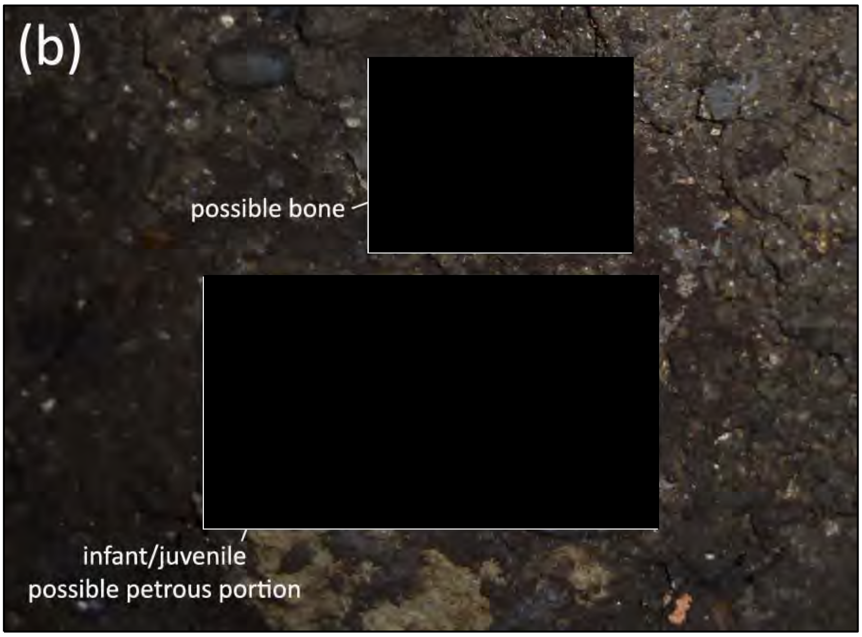


Plate 3.42: C.64/65(b), detail of possible bone and infant/juvenile cranium, see Plate 3.40

Plate 3.43: C.84/85, annotated photograph of sections of identified human remains, see Plates 3.44-3.50

Plate 3.44: C.84/85(a), spread of infant bones, see Plate 3.43 (*n.b.* '?infant petrous portion' refers to the 'infant left temporal' highlighted in Plate 3.45)

Plate 3.45: C.84/85(a), detail, left temporal of infant 0-5 months, see Plate 3.44

Plate 3.46: C.84/85(a), detail, multiple infant bones, including a possibly articulated radius and ulna, see Plate 3.44

Plate 3.47: C.84/85(b), possible infant bones along western edge, see Plate 3.43

Plate 3.48: C.84/85(c), detail of probable infant human bones near south end of tank, see Plate 3.43

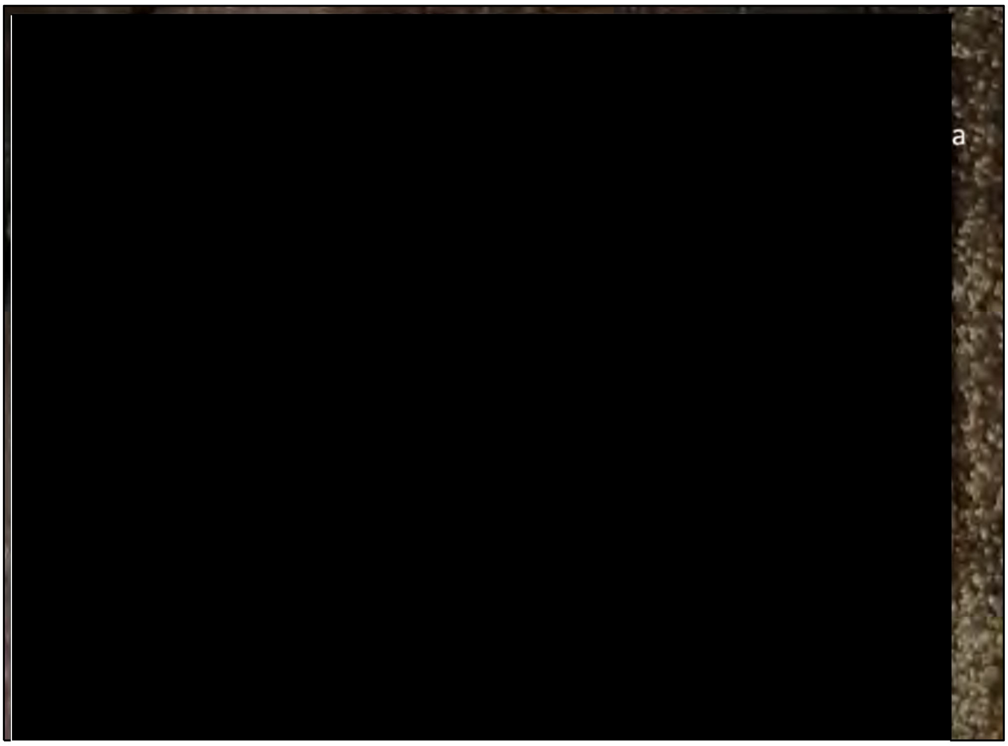


Plate 3.49: C.84/85(c), detail, infant remains with evidence of articulation, see Plate 3.48

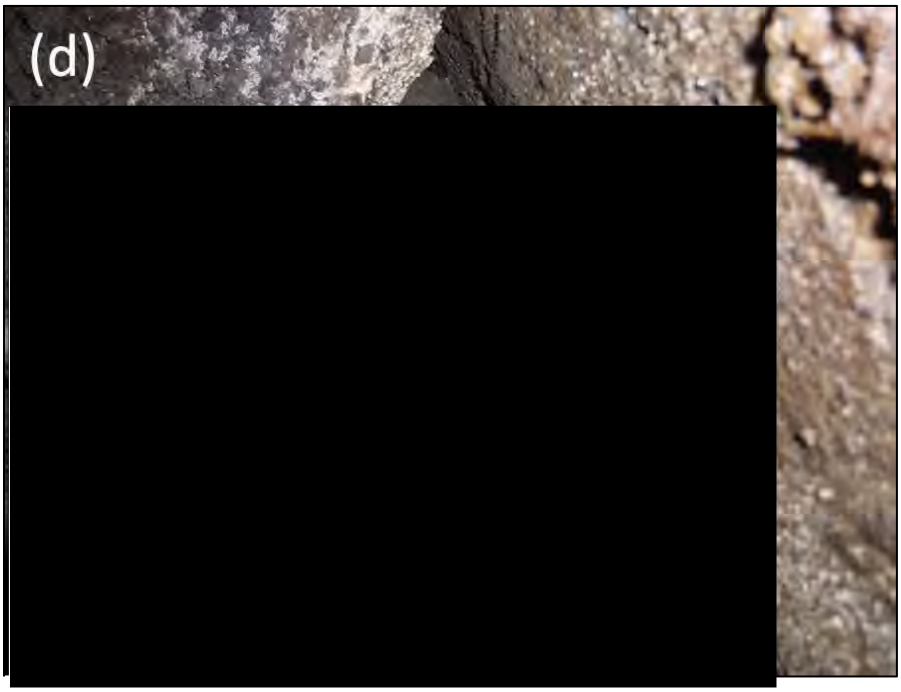


Plate 3.50: C.84/85(d), single possible bone fragment adjacent to east wall, see Plate 3.43

Plate 3.51: C.86/87, no human skeletal remains were visible in this tank

Plate 3.52: C.88/89, annotated photograph of sections of identified human remains, see Plates 3.53-3.60

Plate 3.53: C.88/89(a), multiple bones of infants/young juvenile (<6 years), see Plate 3.52

Plate 3.54: C.88/89(b), multiple bones of infants/young juvenile (<6 years), see Plate 3.52

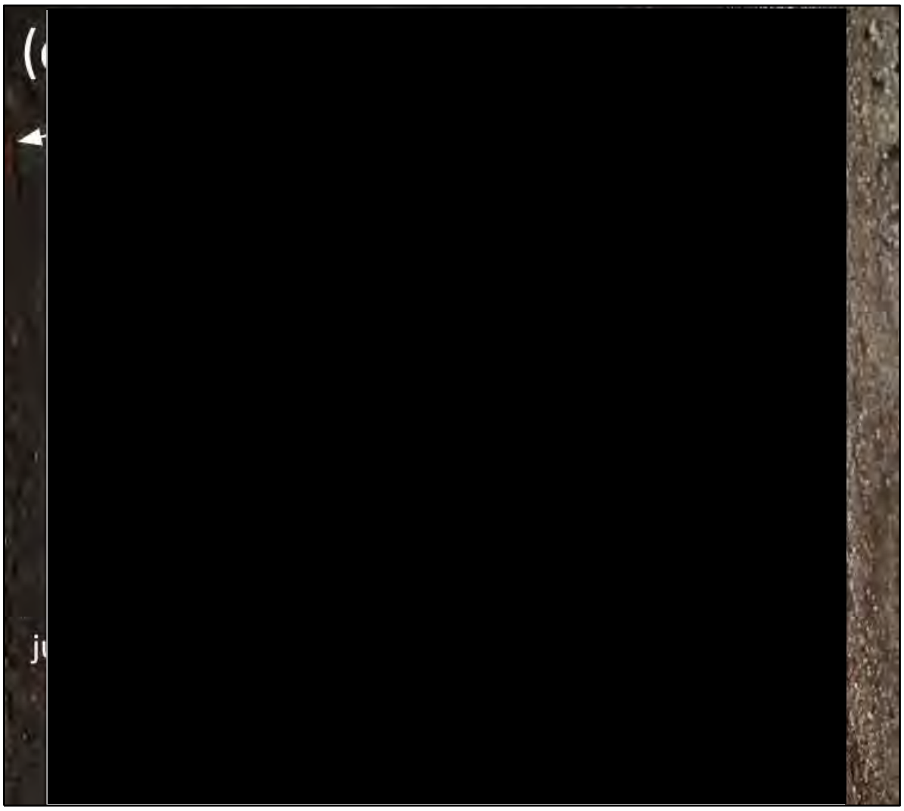


Plate 3.55: C.88/89(c), multiple bones of infants/young juvenile (<6 years), see Plate 3.52

Plate 3.56: C.88/89(d), multiple bones of infants/young juvenile (<6 years), see Plate 3.52

Plate 3.57: C.88/89(e), multiple bones of infants (<1 year) and young juvenile (1.5-2.5 years), see Plate 3.52

Plate 3.58: C.88/89(e), detail, maxillary teeth of disarticulated cranium, with estimated age-at-death of *c.* 1.5-2.5 years, also an infant vertebral arch fragment, north to bottom, see Plate 3.57

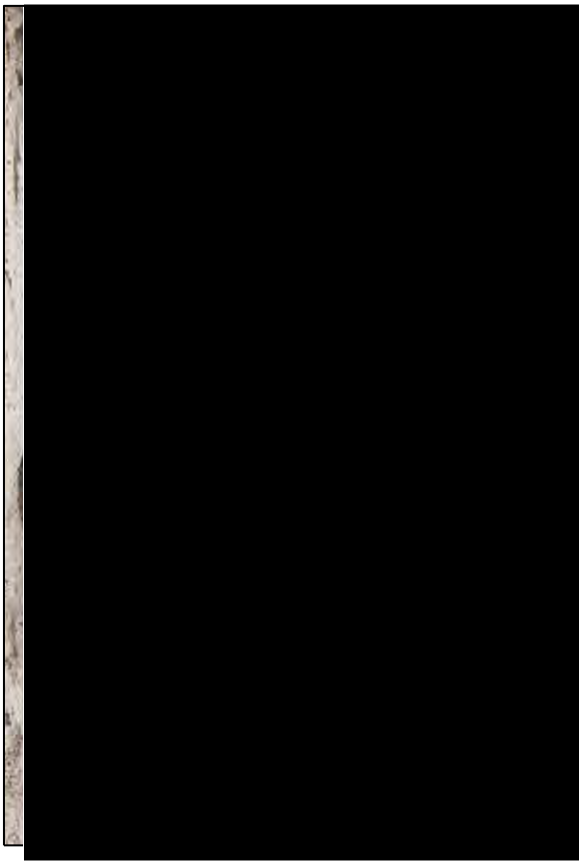


Plate 3.59: C.88/89(e), detail, infant (<1 year) as indicated by humeri, and young juvenile (1-6 years), as indicated by vertebra and cranium, along west side of tank, see Plate 3.57

Plate 3.60: C.88/89(e), detail, infant (<1 year) as indicated by ribs, humerus, and vertebral fragment, and young juvenile (1.5-2.5 years), as indicated by cranium, southwest corner, see Plate 3.57

Plate 3.61: C.90/91, annotated photograph of sections of identified human remains, see Plates 3.62-3.69, and Plate 3.70

Plate 3.62: C.90/91(a), human skeletal remains, see Plate 3.61

Plate 3.63: C.90/91(b), probable infant bones, see Plate 3.61

Plate 3.64: C.90/91(b), detail, showing possible articulation, see Plate 3.61 & 3.63

Plate 3.65: C.90/91(b), detail, showing possible articulation, north to bottom, see Plate 3.61 & 3.63

Plate 3.66: C.90/91(c), infant/juvenile remains near southwest corner, see Plate 3.61

Plate 3.67: C.90/91(c), detail, multiple sets of ribs of infant/young juveniles (<6 years), see Plate 3.66

Plate 3.68: C.90/91(c), detail, right ribs and right scapula of infant/young juvenile (<6 years), detail of Plate 3.67

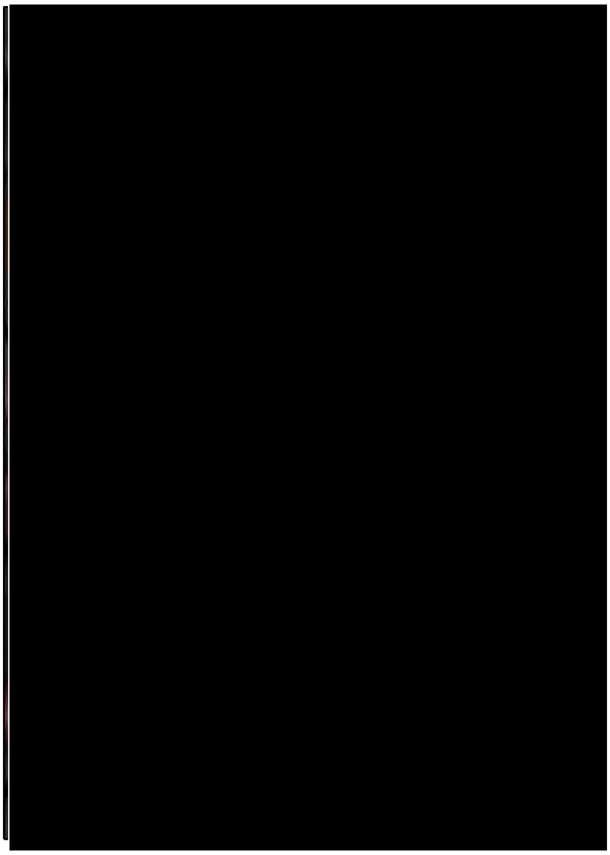


Plate 3.69. C.90/91(c), detail, possibly largely intact cranium of infant/young juvenile (<6 years), detail of Plate 3.67

Plate 3.70: Blue shoe of young juvenile (<6 years), detail from Plate 3.61

Plate 3.71: C.92/93, annotated photograph of sections of identified human remains, see Plates 3.72-3.76

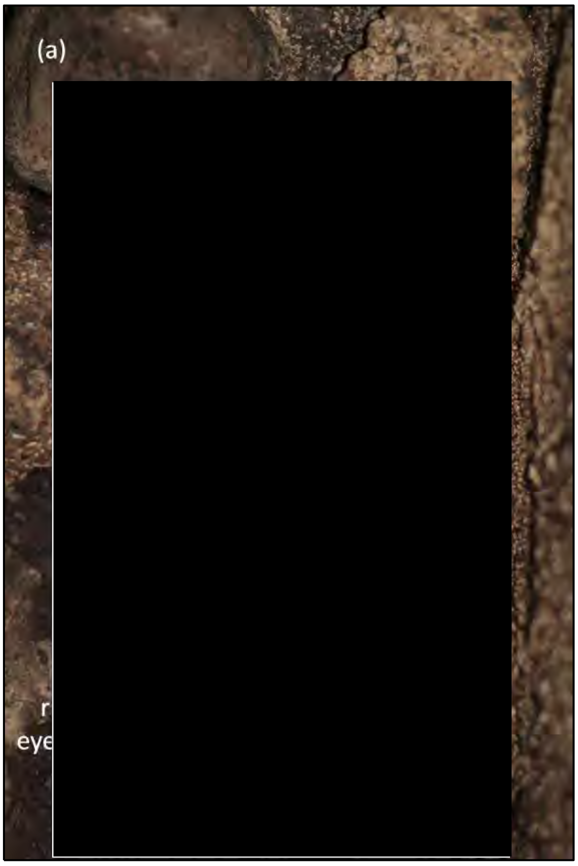


Plate 3.72: C.92/93(a), possibly relatively intact cranium of detail of young juvenile (1-6 years), see Plate 3.71

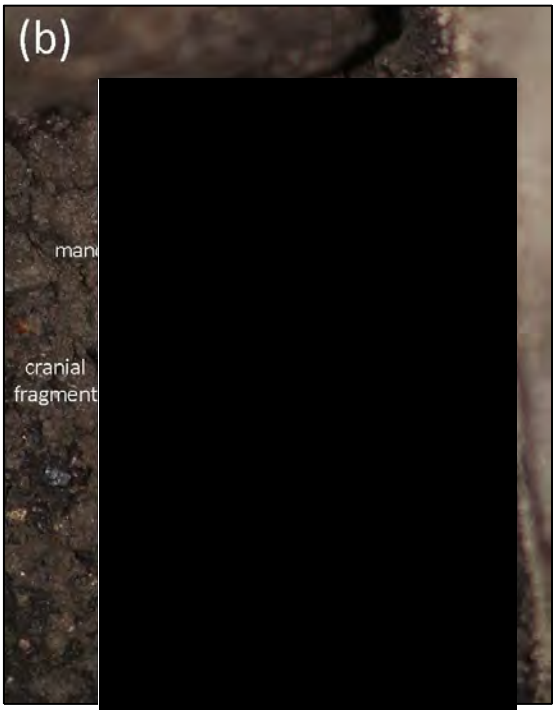


Plate 3.73: C.92/93(b), possible young juvenile (1-6 years) mandible, with cranial fragments and possible hand phalanx, see Plate 3.71

Plate 3.74: C.92/93(c), multiple bones including long bones of juvenile *c.* 2 years, see Plate 3.71

Plate 3.75. C.92/93(d), left ribs and possible scapula of possible young juvenile (1-6 years), see Plate 3.71

Plate 3.76: C.92/93(e), possible cranial fragment, see Plate 3.71

Plate 3.77: C.94/95, annotated photograph of sections of identified human remains, see Plates 3.78-3.83

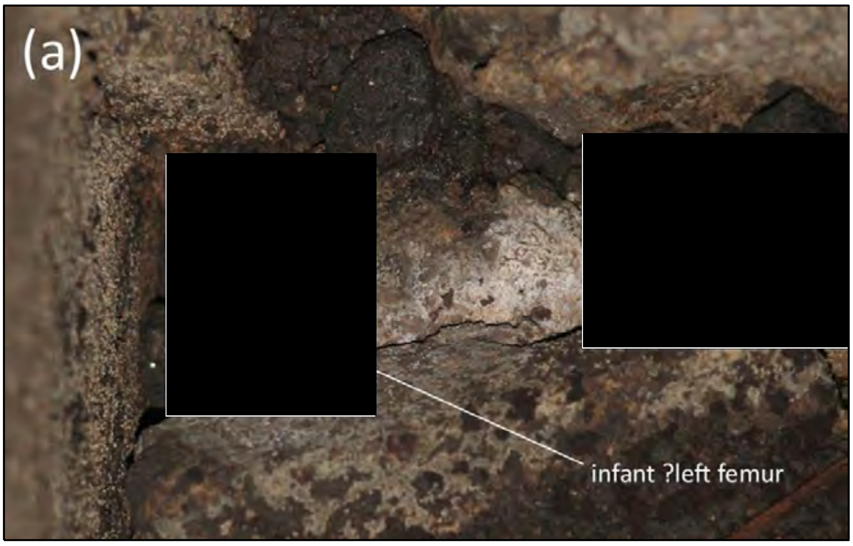


Plate 3.78: C.94/95(a), probable infant left femur, see Plate 3.77

Plate 3.79: C.94/95(b), probable young juvenile (1-6 years) cranium, see Plate 3.77

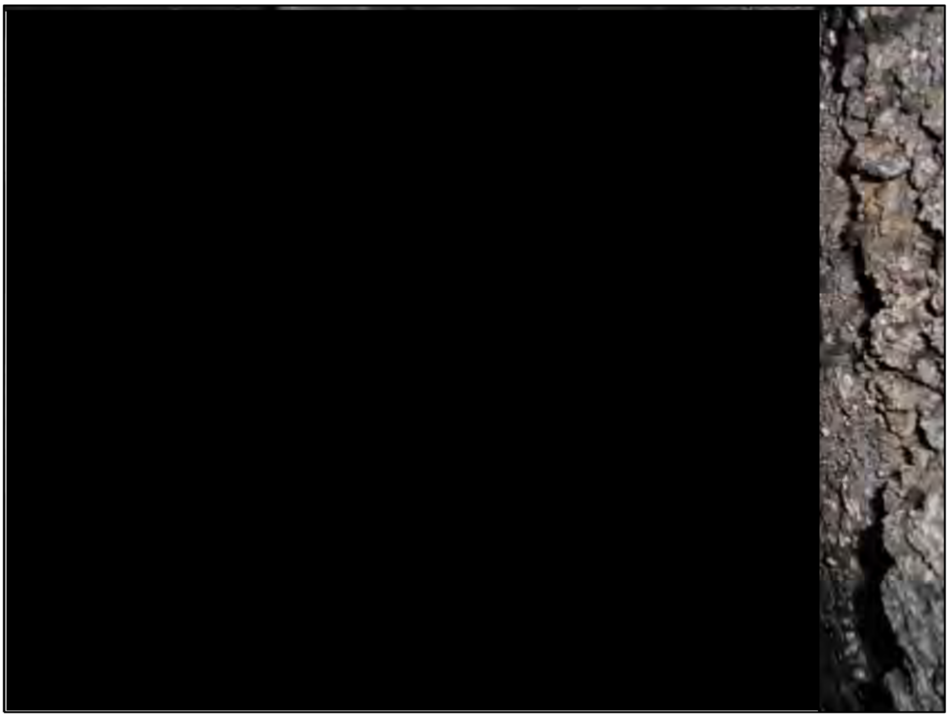


Plate 3.80: C.94/95(c), concentration of probable young juvenile (1-6 years) bones, see Plate 3.77

Plate 3.81: C.94/95(c), detail of unidentified vertebra with at least partial fusion to neural arch, possibly aged 4-6 years, see Plate 3.80

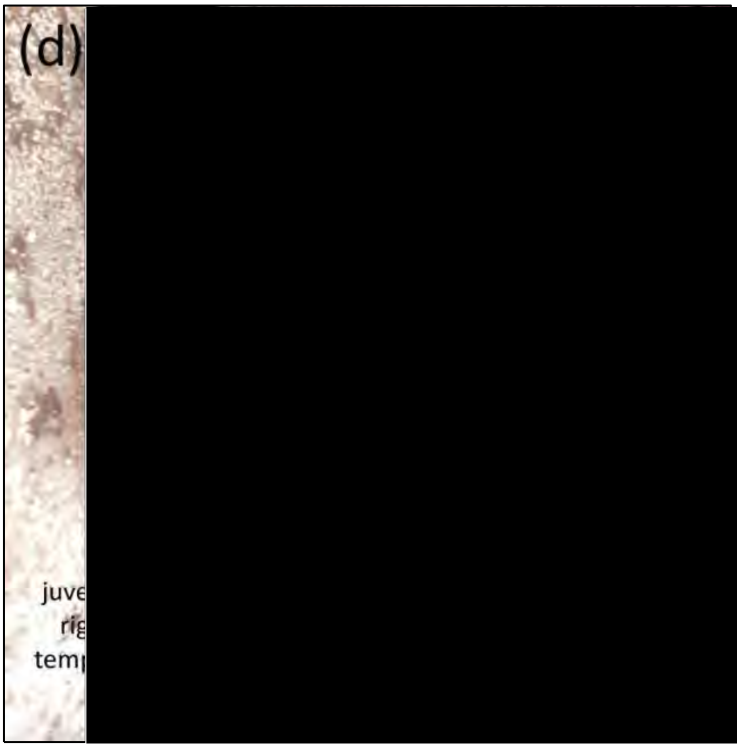


Plate 3.82: C.94/95(d), concentration of young juvenile (1-6 years) cranial bones, see Plate 3.77

Plate 3.83: C.94/95(e), left maxilla of a probable young juvenile (1-6 years), see Plate 3.77


0
0.5m

Plate 3.84: C.96/97, annotated photograph of sections of identified human remains, see Plates 3.85-3.87

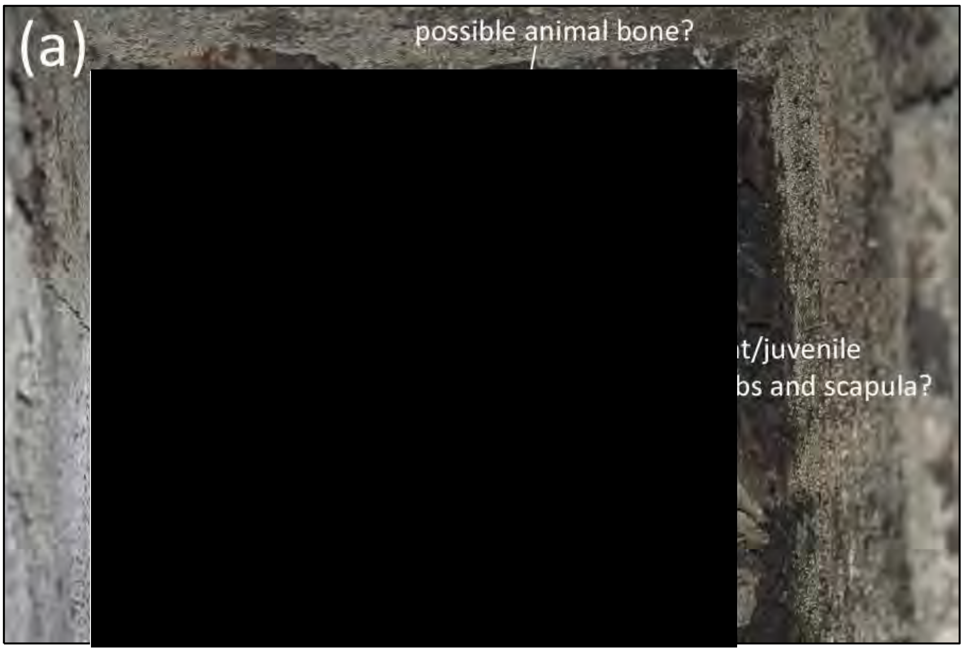


Plate 3.85: C.96/97(a), identified human skeletal remains, see Plate 3.84

Plate 3.86: C.96/97(b), multiple infant bones at south end of tank, see Plate 3.84

Plate 3.87: C.96/97(b), detail, relatively intact infant cranium with possibly associated vertebrae, see Plate 3.86

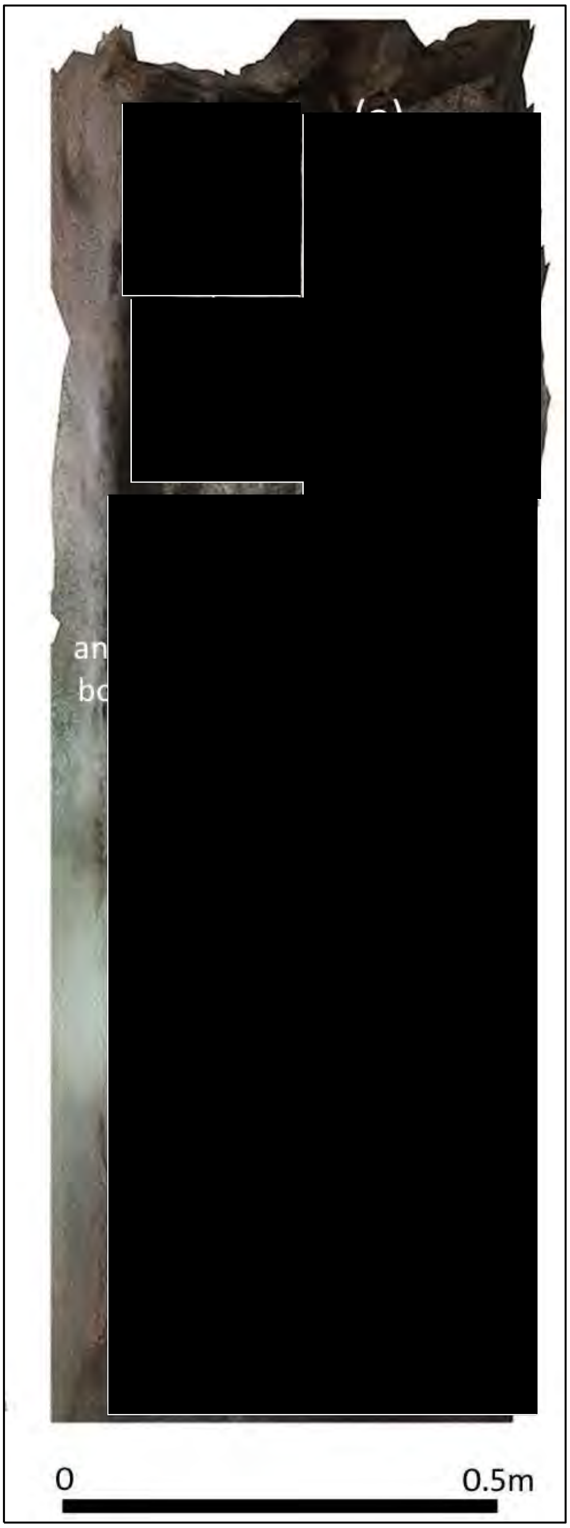


Plate 3.88: C.98/99, annotated photograph of sections of identified human remains, see Plates 3.89-3.91

Plate 3.89: C.98/99(a), possible infant cranial remains at northern end, see Plate 3.88

Plate 3.90: C.98/99(b), possible young juvenile vertebral body, see Plate 3.88

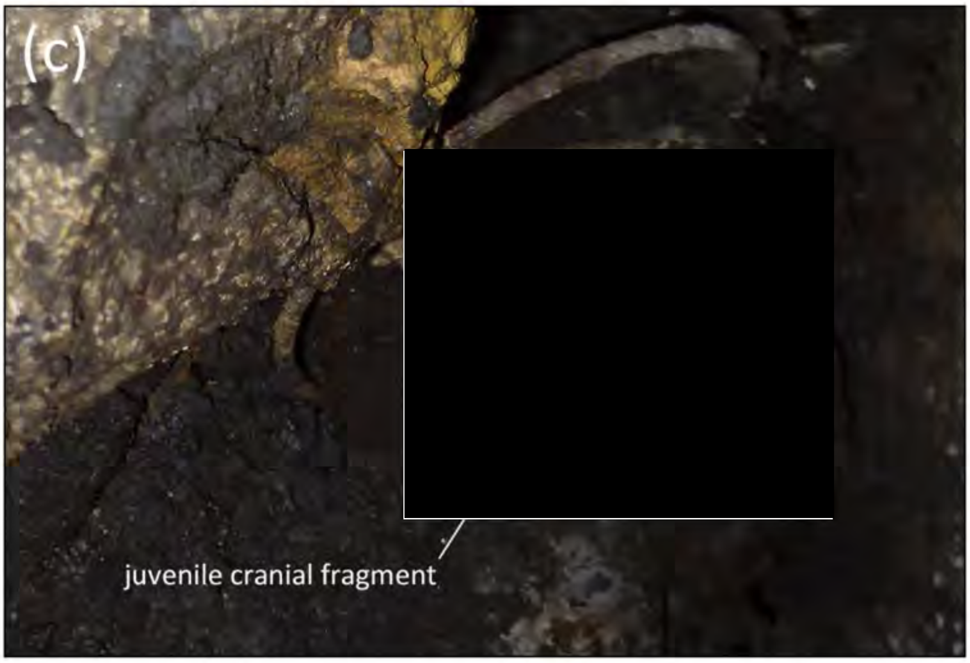


Plate 3.91: C.98/99(c), possible juvenile cranial fragment, see Plate 3.88

Plate 3.92: C.100/101, human remains (a) identified underneath fallen concrete slab, location approximate, see Plates 3.93-3.94

Plate 3.93: C.100/101(a), young juvenile cranial remains underneath collapsed concrete slab, view from north, see Plates 3.92 and 3.94

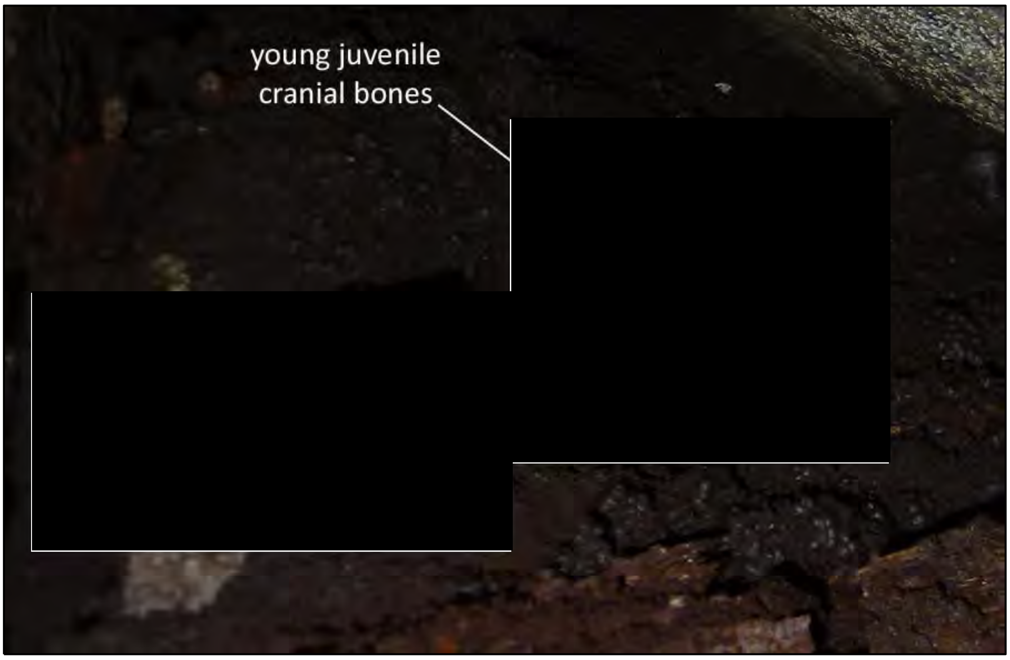


Plate 3.94: C.100/101(a), detail, close up of cranial bones shown in Plate 3.93


Plate 4.1 and 4.2: Castrol Bottle

Plate 4.3: Castrol Logo Chronology, courtesy of BP International

Plate 6.1: Plastic and steel coverings

Plates 6.2: Permeable layer

Plates 6.3: Overburden reinstated

Plates 6.4: Gravel reinstated

Appendix IV: Figures

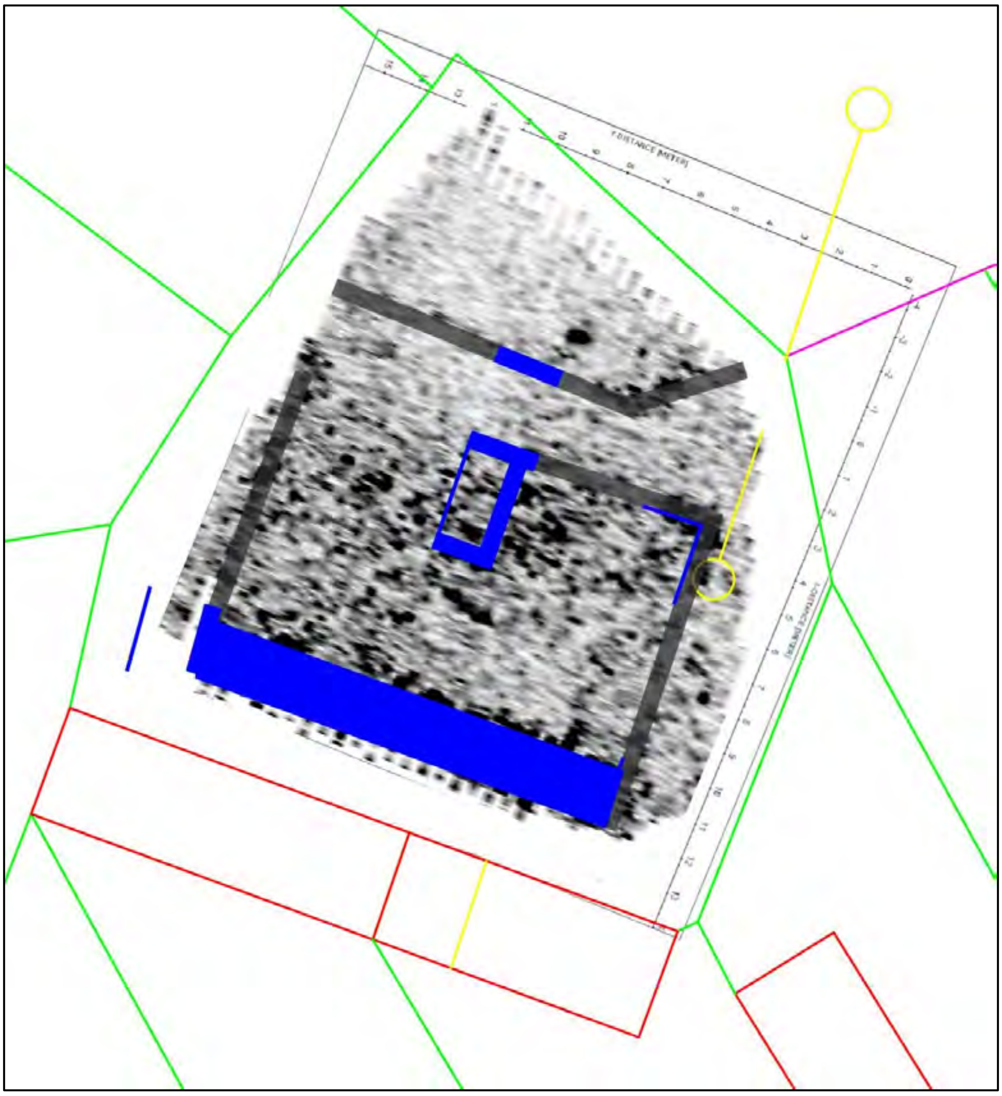


Figure 2.1 Geophysical Survey of the site with the archaeological features identified overlain.

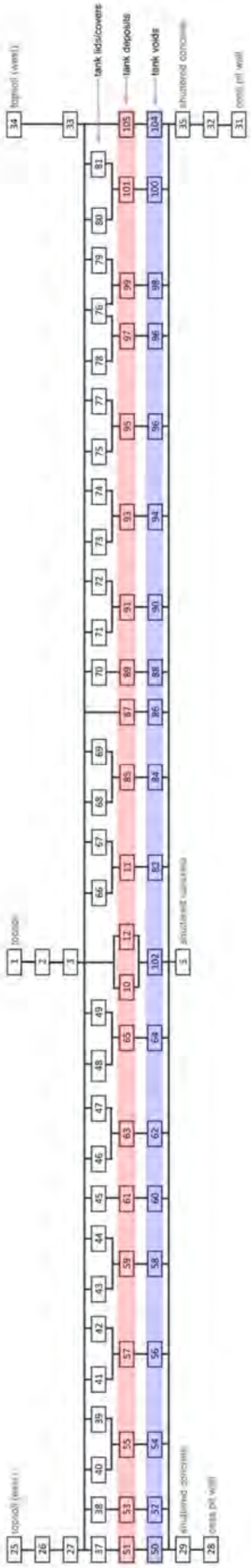
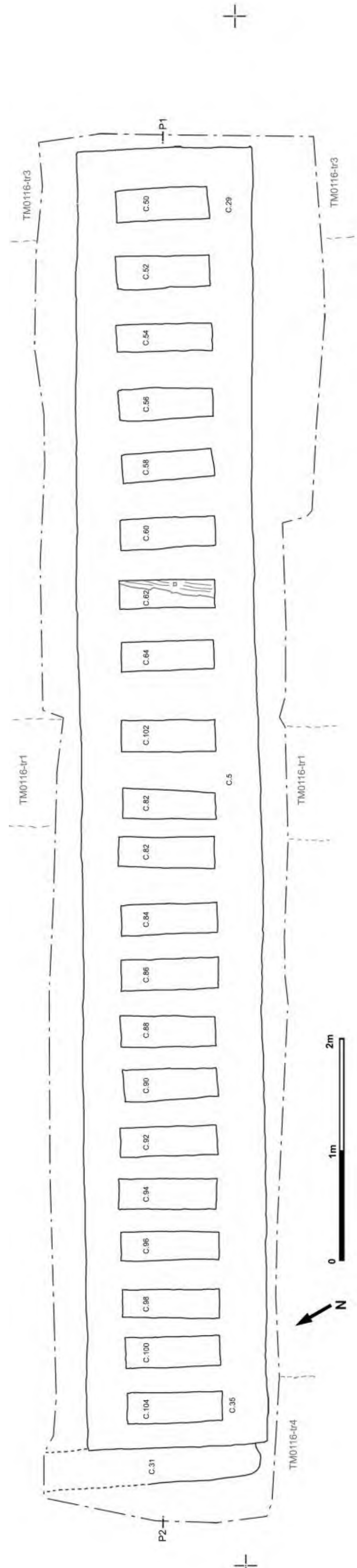


Figure 2.2 Annotated site matrix for Phase IIA

Figure 2.3 and 2.4: Plan and section drawings

of
ope
ning
s



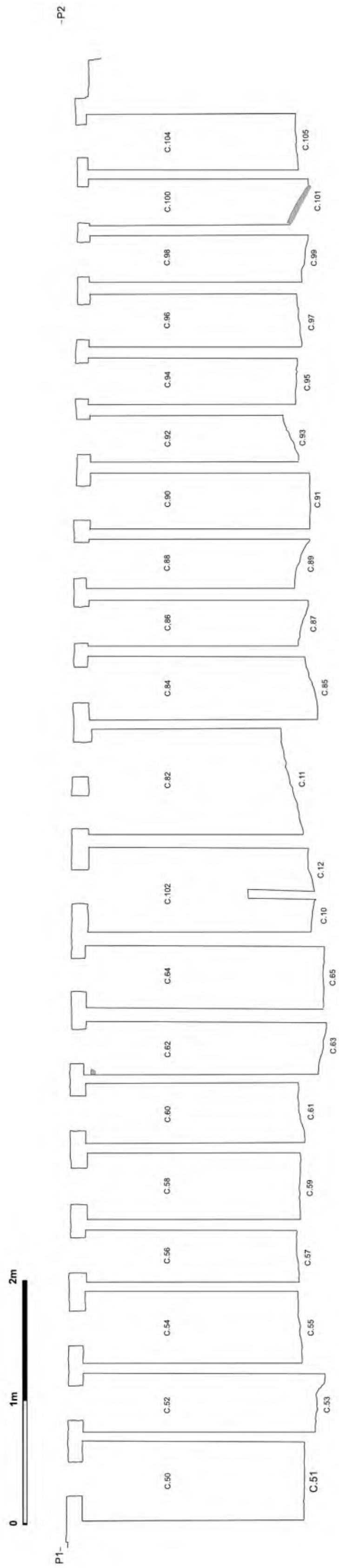


Figure 4.1: C.11/82 illustrating example of debris inserted post deposition of juvenile human remains.

Appendix V: Context Register

MUNSTER ARCHAEOLOGY

Context Register

Site No.:
Site Name: TM1017

Sheet No. 1

Context No.	Type	Area	Description	Plan No.	Date/ Initials
1	Layer	1	Dark brown silt loam, topsoil	2	AH 03/10/16
2	Layer	1	Disturbed greyish brown gravelly/sandy silt, universal extent	2	AH 03/10/16
3	Layer	1	Dark greyish black silt and stone debris	2	AH 04/10/16
5	Masonry	1A	Stone/concrete structure at S end of trench 1 (Feature 1, where F.1A is the eastern tank and F.1B is the western tank)	1, 2, 8	AH 05/10/16
10	Fill/Deposit	1A	Fill of C.5, F.1A eastern-side (not excavated)	-	NMC 07/10/16
11	Fill/Deposit	1A	Fill of C.5, F.1B (not excavated)	-	NMC 07/10/16
12	Fill/Deposit	1A	Fill of C.5, F.1A western-side (not excavated)	-	NMC 07/10/16
25	Layer	3	Dark brown silt loam, topsoil, same as C.1 and C.24	6	MnC 24/10/16
26	Layer	3	Greyish brown sandy silt layer under C.25, equal to C.2 and C.23	6	MnC 24/10/16
27	Layer	3	Dark brownish black layer over concrete shuttering, same as C.3	6	MnC 24/10/16
28	Masonry	3	Short section of limestone wall at NE of trench 3, poss. same as C.21	4	MnC 24/10/16
29	Masonry	3	Stone/concrete shuttered structure with opening (Feature 1 eastern end)	4, 6	AH 26/10/16
31	Masonry	4	Cess-pit wall, mortared limestone, north-south, same as C.21, C.28, C.8 north	7	AH 26/10/16
32	Fill/Deposit	4	Fill of construction trench along W side of C.31	7	AH 26/10/16
33	Layer	4	Greyish brown overburden/backfill	-	AH 26/10/16

MUNSTER ARCHAEOLOGY

Context Register

Sheet No. 2

Site No.:

Site Name: TM1017

Context No.	Type	Area	Description	Plan No.	Date/ Initials
34	Layer	4	Dark brown silt loam topsoil	-	AH 26/10/16
35	Masonry	4	Stone/concrete shuttered structure (Feature 1 western end) with opening to tank	7	AH 26/10/16
37	Masonry	-	Pre-cast concrete slab/lid C.50	-	NMC 31/01/17
38	Masonry	-	Fractured pre-cast concrete slab/lid over C.52	-	NMC 31/01/17
39	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.54	-	NMC 31/01/17
40	Masonry	-	Part of concrete slab/lid-repair (north) over C.54	-	NMC 31/01/17
41	Masonry	-	Part of concrete slab/lid-repair (north) over C.56	-	NMC 31/01/17
42	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.56	-	NMC 31/01/17
43	Masonry	-	Part of concrete slab/lid-repair (north) over C.58	-	NMC 31/01/17
44	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.58	-	NMC 31/01/17
45	Masonry	-	Fractured pre-cast concrete slab/lid over C.60	-	NMC 31/01/17
46	Masonry	-	Part of concrete slab/lid-repair (north) over C.62	-	NMC 31/01/17
47	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.62	-	NMC 31/01/17
48	Masonry	-	Part of concrete slab/lid-repair (north) over C.64	-	NMC 31/01/17
49	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.64	-	NMC 31/01/17

MUNSTER ARCHAEOLOGY

Context Register	Sheet No.
Site No.:	3
Site Name: TM1016	

Context No.	Type	Area	Description	Plan No.	Date/ Initials
50	Void	-	Negative space context within chamber containing fill C.51	-	NMC 31/01/17
51	Deposit	-	Deposit within C.50	-	NMC 31/01/17
52	Void	-	Negative space context within chamber containing fill C.53	-	NMC 31/01/17
53	Deposit	-	Deposit within C.52	-	NMC 31/01/17
54	Void	-	Negative space context within chamber containing fill C.55	-	NMC 31/01/17
55	Deposit	-	Deposit within C.54	-	NMC 31/01/17
56	Void	-	Negative space context within chamber containing fill C.57	-	NMC 31/01/17
57	Deposit	-	Deposit within C.56	-	NMC 31/01/17
58	Void	-	Negative space context within chamber containing fill C.59	-	NMC 31/01/17
59	Deposit	-	Deposit within C.58	-	NMC 31/01/17
60	Void	-	Negative space context within chamber containing fill C.61	-	NMC 31/01/17
61	Deposit	-	Deposit within C.60	-	NMC 31/01/17
62	Void	-	Negative space context within chamber containing fill C.63	-	NMC 31/01/17
63	Deposit	-	Deposit within C.62	-	NMC 31/01/17
64	Void	-	Negative space context within chamber containing fill C.65	-	NMC 31/01/17

MUNSTER ARCHAEOLOGY

Context Register	Sheet No. 4
Site No.:	
Site Name: TM1017	

Context No.	Type	Area	Description	Plan No.	Date/ Initials
65	Deposit	-	Deposit within C.64	-	NMC 31/01/17
66	Masonry	-	Part of fractured pre-cast concrete slab/lid (north) over C.82	-	NMC 02/02/17
67	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.82	-	NMC 02/02/17
68	Masonry	-	Part of concrete slab/lid-repair (north) over C.84	-	NMC 02/02/17
69	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.84	-	NMC 02/02/17
70	Masonry	-	Fractured pre-cast concrete slab/lid over C.88	-	NMC 02/02/17
71	Masonry	-	Part of fractured pre-cast concrete slab/lid (north) over C.90	-	NMC 02/02/17
72	Masonry	-	Part of heavily fractured pre-cast concrete slab/lid (south) over C.90	-	NMC 02/02/17
73	Masonry	-	Part of fractured pre-cast concrete slab/lid (north) over C.92	-	NMC 02/02/17
74	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.92	-	NMC 02/02/17
75	Masonry	-	Concrete slab/lid-repair (north) aligned east-west, over C.94, C.96, C.98 and C.100	-	NMC 02/02/17
76	Metal	-	Corrugated sheeting over C.75	-	NMC 02/02/17
77	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.94	-	NMC 02/02/17
78	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.96	-	NMC 02/02/17
79	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.98	-	NMC 02/02/17

MUNSTER ARCHAEOLOGY

Context Register

Site No.:
Site Name: TM1017

Sheet No. 5

Context No.	Type	Area	Description	Plan No.	Date/ Initials
80	Masonry	-	Concrete slab/lid-repair (north), over C.100	-	NMC 02/02/17
81	Masonry	-	Part of fractured pre-cast concrete slab/lid (south) over C.92	-	NMC 02/02/17
82	Void	-	Negative space context within chamber containing fill C.11	-	NMC 02/02/17
83	Deposit	-	Deposit within C.82, equal to C.11	-	NMC 02/02/17
84	Void	-	Negative space context within chamber containing fill C.85	-	NMC 02/02/17
85	Deposit	-	Deposit within C.84	-	NMC 02/02/17
86	Void	-	Negative space context within chamber containing fill C.87	-	NMC 02/02/17
87	Deposit	-	Deposit within C.86	-	NMC 02/02/17
88	Void	-	Negative space context within chamber containing fill C.89	-	NMC 02/02/17
89	Deposit	-	Deposit within C.88	-	NMC 02/02/17
90	Void	-	Negative space context within chamber containing fill C.91	-	NMC 02/02/17
91	Deposit	-	Deposit within C.90	-	NMC 02/02/17
92	Void	-	Negative space context within chamber containing fill C.93	-	NMC 02/02/17
93	Deposit	-	Deposit within C.92	-	NMC 02/02/17

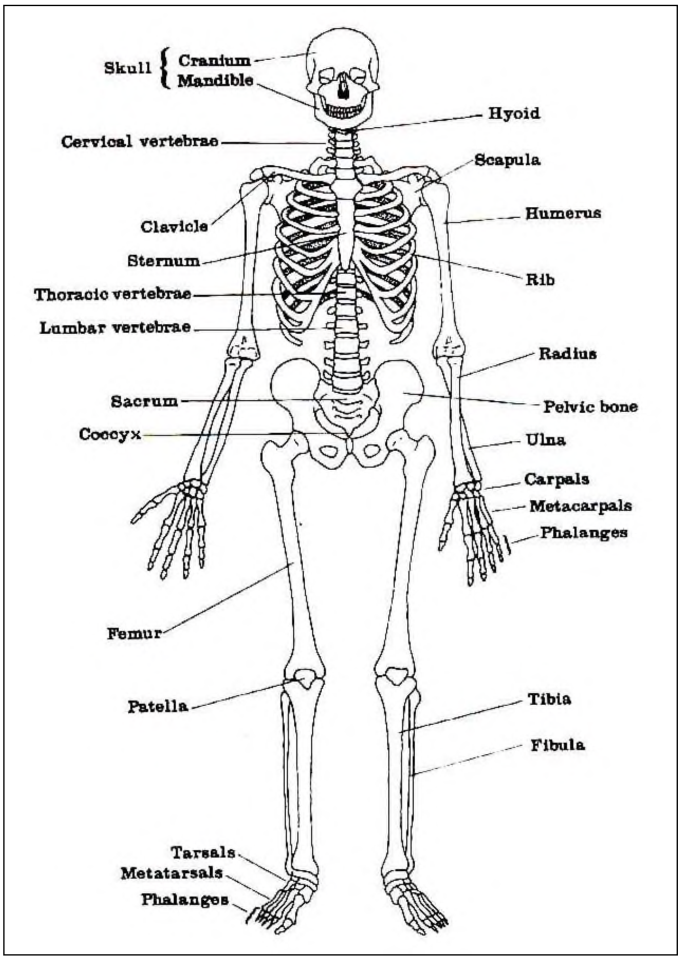
MUNSTER ARCHAEOLOGY

Context Register	Sheet No.
Site No.:	6
Site Name: TM1016	

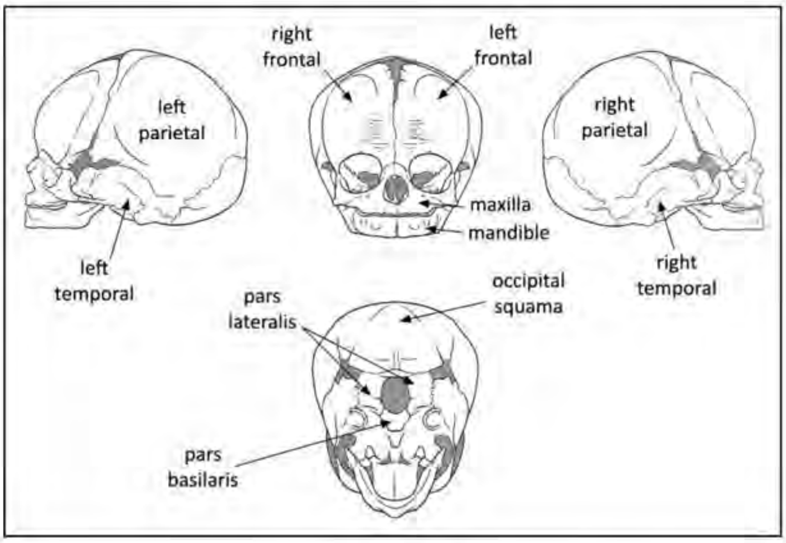
Context No.	Type	Area	Description	Plan No.	Date/ Initials
94	Void	-	Negative space context within chamber containing fill C.95	-	NMC 02/02/17
95	Deposit	-	Deposit within C.94	-	NMC 02/02/17
96	Void	-	Negative space context within chamber containing fill C.97	-	NMC 02/02/17
97	Deposit	-	Deposit within C.96	-	NMC 02/02/17
98	Void	-	Negative space context within chamber containing fill C.99	-	NMC 02/02/17
99	Deposit	-	Deposit within C.98	-	NMC 02/02/17
100	Void	-	Negative space context within chamber containing fill C.101	-	NMC 02/02/17
101	Deposit	-	Deposit within C.100	-	NMC 02/02/17
102	Void	-	Negative space context within chamber containing fills C.10 and C.12	-	NMC 02/02/17
104	Void	-	Negative space context within chamber containing fill C.105	-	NMC 02/02/17
105	Deposit	-	Deposit within C.104	-	NMC 02/02/17

Appendix VI: Osteological Appendices

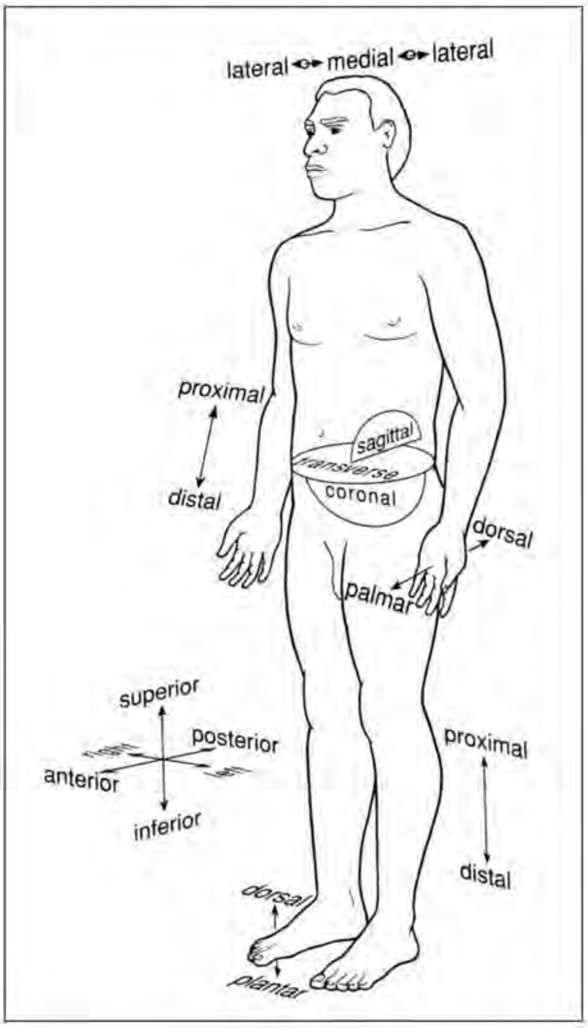
A. Annotated diagram showing main skeletal elements (after Mays 1998, 2, fig. 1.1)



B. Annotated diagram showing main elements of infant cranium (adapted from Schaefer et al. 2009, 360)



C. Anatomical directions(from White and Folkens 1991, 29, fig. 3.1)



D. Osteological Terms Used (after White and Folkens 1991, 28-35; Bass 1995, 319-321)

Directions - General

Superior	toward the head of the body.
Inferior	opposite of superior, body parts away from the head.
Anterior	toward the front of the body.
Posterior	opposite of anterior, toward the back of the individual.
Medial	toward the midline of the body.
Lateral	opposite of medial, away from the midline of the body.
Proximal	nearest the axial skeleton, usually used for long bones.
Distal	opposite of proximal, furthest from the axial skeleton.
Palmar	relating to the hand, the palm side
Plantar	relating to the foot, towards the sole of the foot
Dorsal	relating to the hand/foot, back of the hand, top side of the foot
External	outer.
Internal	opposite of external, inside.
Endocranial	inner surface of the cranial vault.
Ectocranial	outer surface of the cranial vault.

Directions - Teeth

Mesial	toward the point on the midline where the central incisors meet.
Distal	opposite of mesial.
Lingual -	toward the tongue.
Labial	opposite of lingual, toward the lips.
Buccal	opposite of lingual, toward the cheeks.
Incisal	the biting surface of the tooth.
Occlusal	the chewing surface of the tooth.

General bone features/terms

Process	a bony eminence.
Eminence	a bony projection, usually not as prominent as a process.
Spine	generally a long, thinner, sharper process than an eminence.
Tuberosity	a large, usually roughened eminence of variable shape, often the site of a ligament attachment.
Tubercle	a small, usually roughened eminence, often a site of a ligament attachment.
Trochanters	two large, prominent, blunt, rugose processes found on the distal femur.
Malleolus	a rounded protuberance adjacent to the ankle joint.
Articulation	an area in which adjacent bones are in contact at a joint.
Condyle	a rounded articular process.
Epicondyle	a non-articular projection adjacent to a condyle.
Head	a large, rounded, usually articular end of a bone.
Shaft/diaphysis	the long, straight section between the ends of a long bone.
Epiphysis	usually the end portion or extremity of a long bone which is expanded for articulation.

Neck	the section of a bone between the head and the shaft.
Torus -	a bony thickening.
Ridge	a linear bony elevation, often roughened.
Crest	a prominent, usually sharp and thin ridge of bone.
Line	a raised linear surface, not as thick as a torus or as sharp as a crest.
Facet	a small articular surface, or tooth contact.
Metaphysis	a line of junction between epiphysis and diaphysis.
Osteoblastic	process of bone formation
Osteoclastic	process of bone resorption

Other osteological terms/abbreviations

C1-C7	cervical vertebrae (neck) numbered from 1-7.
CEJ	cemento-enamel junction, junction of crown of tooth and root.
DJD	degenerative joint disease.
T1-T12	thoracic vertebrae (torso) numbered 1-12.
TMJ	tempromandibular joint, joint of lower jaw.
L1-L5	lumbar vertebrae (lower back) numbered 1-5.
S1-S5	sacral vertebrae (in between left and right pelvis) numbered 1-5.
MC-	metacarpal (bones of the palm of the hand), may be numbered 1-5.
MT	metatarsal (bones of the arch of the foot), may be numbered 1-5.
IAM	Internal Auditory Meatus in temporal bone of cranium.
EAM	External Auditory Meatus in temporal bone of cranium.
MN	Minimum Number of Individuals.
CPR	Crude Prevalence Rate.
TPR	True Prevalence Rate.
SN/s	Schmorl's nodes, depression defects in the vertebral bodies, associated with herniation of intervertebral disk.

Appendix VII: Environmental Sampling Report

Joint Report
The Characterisation of Samples
For Niamh McCullagh and
The Mother and Baby Homes Commission of Investigation

(Criminal Procedure Rules [2015] Parts 16 and 19; Criminal Justice Act 1967, s. 9)

Report of Professor Lorna DAWSON, Dr Tom SHEPHERD and Dr Bob MAYES

Qualifications
BSc, PhD, C.Sci, F.I.Soil Sci, FRSA (LD);
BSc, PhD (TS);
BSc, MSc, PhD (BM),

Age Over 18

Occupations Soil Scientist, Volatile Organic Chemist and Organic Chemist

Address James Hutton Institute
Craigiebuckler
Aberdeen
AB15 8QH

I (Lorna DAWSON, Tom SHEPHERD and Bob MAYES) DECLARE THAT:

1. I understand that my duty is to help the court to achieve the overriding objective by giving independent assistance by way of objective, unbiased opinion on matters within my expertise, both in preparing reports and giving oral evidence. I understand that this duty overrides any obligation to the party by whom I am engaged or the person who has paid or is liable to pay me. I confirm that I have complied with and will continue to comply with that duty.

2. I confirm that I have not entered into any arrangement where the amount or payment of my fees is in any way dependent on the outcome of the case.

3. I know of no conflict of interest of any kind, other than any which I have disclosed in my report.

4. I do not consider that any interest which I have disclosed affects my suitability as an expert witness on any issues on which I have given evidence.

5. I will advise the party by whom I am instructed if, between the date of my report and the trial, there is any change in circumstances which affect my answers to points 3 and 4 above.

6. I have shown the sources of all information I have used.

7. I have exercised reasonable care and skill in order to be accurate and complete in preparing this report.

8. I have endeavoured to include in my report those matters, of which I have knowledge or of which I have been made aware, that might adversely affect the validity of my opinion. I have clearly stated any qualifications to my opinion.

9. I have not, without forming an independent view, included or excluded anything which has been suggested to me by others including my instructing lawyers.

10. I will notify those instructing me immediately and confirm in writing if for any reason my existing report requires any correction or qualification.

11. I understand that:

    (a) my report will form the evidence to be given under oath or affirmation;

    (b) the court may at any stage direct a discussion to take place between experts;

    (c) the court may direct that, following a discussion between the experts, a statement should be prepared showing those issues which are agreed and those issues which are not agreed, together with the reasons;

    (d) I may be required to attend court to be cross-examined on my report by a cross-examiner assisted by an expert.

    (e) I am likely to be the subject of public adverse criticism by the judge if the Court concludes that I have not taken reasonable care in trying to meet the standards set out above.

12. I have read Part 19 of the Criminal Procedure Rules and I have complied with its requirements.

13. I confirm that my discipline does not have a material code to adhere to.

14. I confirm that I have read guidance contained in a booklet known as *Disclosure: Experts' Evidence and Unused Material* which details my role and documents my responsibilities, in relation to revelation as an expert witness. I have followed the guidance and recognise the continuing nature of my responsibilities of disclosure. In accordance with my duties of disclosure, as documented in the guidance booklet, I confirm that:

    (a) I have complied with my duties to record, retain and reveal material in accordance with the Criminal Procedure and Investigations Act 1996, as amended;

    (b) I have compiled an Index of all material. I will ensure that the Index is updated in the event I am provided with or generate additional material;

    (c) in the event my opinion changes on any material issue, I will inform the investigating officer, as soon as reasonably practicable and give reasons.

I confirm that the contents of this report are true to the best of my knowledge and belief and that I make this report knowing that, if it is tendered in evidence, I would be liable to prosecution if I have wilfully stated anything which I know to be false or that I do not believe to be true.

Signed Dated the 23rd May 2017

Signed Dated the 23rd May 2017

Signed Dated the 23rd May 2017

Table of Contents

1. Qualifications and Experience

Prof. Lorna DAWSON

I am employed as a principal research scientist at the James Hutton Institute, Aberdeen, Scotland, where I am Head of the Soil Forensics Section and hold the qualifications of BSc (Honours) Geography (Edinburgh University, 1979), and a PhD in Soil Science (Aberdeen University, 1984). I am a visiting Professor in Forensic Science at the Robert Gordon University. I am a Fellow of the British Society of Soil Science, a Fellow of the Royal Society of the Arts, a Chartered Scientist and hold an Expert Witness certificate in both Criminal and Civil Law (Cardiff University, 2011, 2012). I have published widely on the subject of forensic soil science; published over 80 refereed publications, books and book chapters. I am an Expert Advisor with the National Crime Agency, have worked with numerous police forces in Scotland, England, Wales, Ireland & Australia over the last 12 years and have advised on over 100 cases, written over 70 Expert Witness reports, and presented evidence in 10, in the UK and overseas. During the past 12 years I have encountered the evidence type involved in this case on several occasions.

Dr Tom SHEPHERD

I am a senior research chemist employed at the James Hutton Institute, Dundee, Scotland holding the qualifications of BSc (Honours) Chemistry (University of St Andrews, 1980) and a PhD in Synthetic Organic Chemistry (University of St Andrews, 1983). I am an expert in the use of techniques such as automated thermal desorption (ATD) and solid-phase micro-extraction (SPME), coupled with GC-MS, for entrainment and analysis of volatiles. A main element of my research is the analysis of volatile chemicals, compiling an extensive database of chromatographic characteristics from a wide range of different matrices. During the past two years I have encountered the evidence type involved in this case on several occasions.

Dr Bob MAYES

I am a Research Associate at the James Hutton Institute where I was previously head of the Ecological Sciences GC and GC-MS laboratories, and hold the qualifications PhD from Queen's University of Belfast, MSc in Animal Nutrition from the University of Aberdeen and BSc in Physiology and Biochemistry of Farm Animals from Reading University. I am an expert in the analysis of wax markers and my research interests revolve around the application of this biomarker technology to measuring dietary intake, digestibility and plant species composition in grazing herbivores and to the chemical characterisation of soil organic matter as applied in criminal investigations. I have worked with a number of police forces in Scotland, England, Wales & Ireland over the last 6 years, have written over 16 Expert Witness reports, and presented evidence in court with two of them. During the past 6 years I have encountered the evidence type involved in this case on several occasions.

2. Summary of findings

- It can be confirmed from our examination that there is evidence that the site *had* previously been used as a sewage facility.
- The results of this series of tests cannot establish categorically whether the sewage facility was being used at the time when the human remains were deposited. It is a matter of historic record to establish when and how long the facility was used.
- The results of this series of tests cannot establish categorically whether the non-decomposed human remains had been deposited in the chambers, or whether the bodies have previously been stored (and decomposed) elsewhere, with mainly bones being placed in the chambers.

It does appear that the volatile organic profiles are characteristic of decomposition of mammalian tissue *or* waste and probably human. It is not possible to determine the extent to which the deposited human infant remains which are known to be present may have contributed to this, or to what extent human faecal material may also have done so. The presence of hotspots within the northern and western boundary samples but not the southern and eastern boundary samples is of note. A number of the hotspots for compounds characteristic of bone decomposition, particularly ketones, but also aliphatic alcohols and *n*-aldehydes, are found at locations with high bone densities.

However, the concentrations of the solid organic biomarkers in the analysed samples were very low, much lower than would be expected if the analysed material had entirely originated from human sewage waste. The samples collected from the site boundaries (negative control samples; samples 55 and 57) had generally lower biomarker concentrations than the samples collected from within the chambers where remains were located. 10-Hydroxy stearic acid, cholesterol and the faecal stanols, coprostanol and epicoprostanol have been recognised as being products of the decomposition of mammalian remains (including human), and their concentration patterns generally differ from those of human sewage material. The presence of these compounds in the samples collected from the chambers could, at least in part, have come from decomposed human bodies.

The reasons for the low biomarker concentrations found in the samples are not easy to assess. If the chambers represented a closed cesspit or a number of cesspits, it is possible that the collected sewage had been removed before depositing the human cadaver material; soil may have been added at the same time, or soil may have seeped in from the roof area of the chambers. If there were one or more piped out flows (i.e. the facility was a septic tank, or was connected to a sewer outflow), it would be expected that little sewage would be left behind.

Samples 55 and 57 (west boundary and east boundary locations respectively) and sample 14 (no visible human remains) have different isotopic profiles to the other samples examined, reflecting likely a lesser influence from either sewage or human remains.

It is likely that some signature due to faecal material is present, but it is also likely that the human remains have also contributed to the signatures observed, and the presence of compounds associated with decomposition of bone at locations of high bone density in the samples is suggestive of this.

3. Information/Circumstances of Case

We examined a single sample of soil (DAWSON & MAYES Report dated 6th December 2016) and ascertained that that sample was not a typical soil but was shown to contain faecal markers and potential indications of human decomposition markers.

I, Lorna DAWSON, later received a phone call from Donal GUINNESS, Counsel to the Mother and Baby Home Commission of Investigation, on 7th February, 2017 to enquire if we could carry out a set of Volatile Organic Compound (VOC) analyses of 20 soil samples, followed by an independent alkane/sterol/alcohol analysis on the interesting samples as identified from the initial VOC analysis. After discussion with Niamh McCULLAGH, forensic archaeologist, and representing the Counsel to the Mother and Baby Home Commission of Investigation, a tender with agreed costs for VOC screening of 32 samples, followed by detailed VOC interpretation and alkane/sterol/alcohol analysis of 6 interesting samples was sent on 13th February 2017, the work having been commissioned on the 12th February 2017.

The conclusions we have drawn in this case are based on information provided by Niamh McCULLAGH. Should this information change it may be necessary for us to reconsider our interpretation and conclusions.

4. Items Received

A scanned copy of the list of samples collected at the site under investigation is in Appendix 1. Samples were taken from several locations in a rectangular facility with several concrete cells within that outer structure (and is described in a separate report by McCULLAGH) Appendix 10. Two samples were taken at each location, one of which was retained by the client. All samples not marked as retained were delivered by DHL couriers to the James Hutton Institute, Aberdeen on the 15th February 2017 in a sealed box. Inside the sealed box was a second box securely sealed on all edges containing 2 sealed evidence bags MRHC01 – bags 1 & 2.

5. Request or Purpose of Examination

Human remains have been found within a structure at a site that, in general terms, has been used previously as a sewage treatment facility. The investigative questions relevant to the sample submissions are:

a) Can it be determined if the structure from which human remains were recovered was or ever had been used as a sewage treatment facility?
b) Can it be determined if this structure was in use at the time remains were deposited?

c) Can it be determined if these remains decomposed in situ? If so, what degree of certainty can be applied to the result?

6. Assumptions

It is assumed the samples were collected in a rigorous manner and that the sampling was carried out with due care and by adhering to established forensic sampling protocols.

7. Use of Assistants

In undertaking the work in this case I, Lorna DAWSON was assisted by other members of the Soil Forensic Unit Laboratory staff. Their involvement is described in the forensic case files and I have taken their contributions into account when we prepared this report. The involvement of other staff is fully recorded in case notes available for inspection at the laboratory if necessary. Mrs Jasmine ROSS, forensic laboratory manager, assisted myself in examining the samples, captured photographs, analysed the samples for organic markers and prepared the audit trail (Appendix 2). Dr Tom SHEPHERD analysed the samples for VOCs by Solid Phase Microextraction - Gas Chromatography – Mass Spectrometry (SPME-GC-MS) and interpreted the VOC data. Dr Bob MAYES interpreted the organic marker chromatograms for markers of sewage and or human decomposition. Mrs Maureen PROCEE analysed the samples for isotopic C and N. Mr Gareth NEWMAN, Service Delivery Manager, James Hutton Limited, carried out a stage 1 review of this report. Prof. Colin CAMPBELL, CEO, James Hutton Institute, reviewed this report.

8. Nature of Examination

Soil is a mixture of both inorganic and organic material (Dawson and Hillier, 2010: Dawson and Mayes, 2014). The organic material reflects the plant and animal material having been deposited or decomposed within that soil and also human organic inputs to the soil (Dawson and Mayes, 2014). A combination of gas chromatography (GC) and gas chromatography-mass spectrometry (GCMS) can be used to characterise and identify many organic compounds in soils, both volatile and physical which helps ascertain what those inputs likely were.

Comparison of the distribution of the volatile compounds found in the samples with published data describing the range of volatile compounds produced during decomposition of mammalian tissues, including that of humans (Vaas et al., 2004, 2008; Vaas, 2012) allows the interpretation of contact with human decomposition products to be made. This use of the examination of the odour of decomposition is relatively recent and is considered an experimental technique for intelligence and is still under development.

This report describes the sample examination, the VOC analysis, the organic analysis and the isotope analysis of the samples received on the 15th February 2017.

A full record of the work done in this case is available for inspection at Laboratory 234, the James Hutton Institute, Aberdeen.

An audit trail is in Appendix 2. A list of references used is in Appendix 3. Materials and methods for VOCs, low volatility organic compounds and isotope analysis are in Appendices 4, 5 and 6.

9. Results

Selection of the eight most interesting samples for further analysis

From the phase 1 VOC analysis results, interesting samples were selected for examination for non-volatile organic marker analysis (Table 1, page 10). In addition to the samples identified by the VOC analysis a further 3 samples were chosen for analysis. These were: sample 18 (C.65) where no human remains were seen, sample 35 (C.91) where a fragment of bone was seen when the sample was taken, and sample 57 (east boundary) as a negative control that contained low levels of VOCs.

For every sample, the abundances of individual components in each of the 16 different compound classes were combined to give a compound class sum. Compound class sums for each sample were combined to give a compound class total across all samples.

The compound class sums for each sample were then expressed as a percentage of the compound class total across all samples. This is the scaled abundance. For an individual compound class the sum of the scaled abundances across all samples is 100 (rows in the table).The scaled abundances for the individual compound classes in each individual sample were then combined (columns in the table) to give a combined scale abundance score for the sample

Samples were ranked according to their combined scale abundance scores (in the line below main table), and the eight samples with the highest scores were identified (in grey on right hand side of table): (samples 055, 049, 007, 001, 011, 014, 005 and 045).

Table 1. Compound class analysis for identification of samples with interesting profiles for further analysis based on amounts of classes of compounds of interest. First key refers to individual abundances within main table and second key refers to sum of compound classes.

Sample Numbers (Context Numbers) — Bulk Boundary Controls (53–59)

Compound Class	1	3	5	7	9	11	13	14	15	17	18	19	21	23	25	27	29	30	31	33	35	37	39	43	45	47	49	51	53	55	57	59
	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	N	W	E	S
Aliphatic Alcohols	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Aromatic Alcohols	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Phenols	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Sulfur compounds	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Aliphatic Ketones	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Aromatic Ketones	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Halocarbons	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Furans	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Branched Aldehydes	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Aromatic Aldehydes	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
n-Aldehydes	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Aromatic Hydrocarbons	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Aliphatic Acids	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Aromatic Acids	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Unsaturated Aldehydes	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
Alkanes	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

0-3
3-6
6-9
9-12
12-15
15 - 20
20 - 40

Distribution of individual compound classes across all samples expressed as a percentage of their combined total abundance for each compound class

(sum of horizontal rows = 100)

Scaled Abundance Scores For Individual Compound Classes

10-20
20-40
40-60
60-100
100 - 150
150+

Combined scaled abundance scores per sample for all compound classes

(sum of vertical columns)

Samples (n = 8) with the highest combined scores

Signature ....Page 10 of 103

Soil description

Sub-samples of the 11 selected interesting samples were taken and dried overnight at 40° C before being photographed under a Nikon SMZ1500 binocular microscope at either times 10 or times 20 magnification. Images are in Appendix 9.The sub-samples were then hand ground with an agate mortar and pestle before weighing for organic biomarker analysis by GC and GCMS.

Table 2. Description of samples examined.

Exhibit/Item Number	**Location**	**Context**	**Mineral Composition**	**Organic material and other fragments**	**Density of remains** (from osteologist's report as provided by Niamh McCULLAGH)
Sample 1	C.50 Z1 20cm to 'gravel'.	C.51	No stones. Small white grains.	No discrete vegetation. White/yellow material.	High
Sample 5	C.54 Z6 25cm to 'gravel'.	C.55	Few medium stones. White stones, quartz grains.	Highly organic. Reddish/orange organic material. Material which could be bone seen at X10 magnification.	Medium, animal bone also visible.
Sample 7	C.56 Z1	C.57	No stones. White quartz grains.	Highly organic. Orange/white material. Material which could be bone seen at X10 magnification.	High
Sample 11	C.60 Z6 12cm to 'gravel'.	C.61	Fine textured. Very small stones and quartz grains. Crystallized material.	Highly organic. Material which could be bone seen at X10 magnification.	Medium

Sample 14	C.62 Z7 No HR visible 4cm to 'gravel'.	C.63	Fine textured. Quartz grains and spherical clear particles.	Highly organic. Yellow/white material.	No HR visible.
Sample 18	C.64 Z7 14cm to 'gravel'.	C.65	Fine textured. Quartz grains and very small stones. Brick. Black coal type material.	Highly organic.	Low
Sample 35	C.90 Z5 25cm to 'gravel' includes bone.	C.91	Fine textured. Small stones and quartz grains.	Flaky orange/brown material (bone?). Material which could be bone seen at X10 magnification.	High
Sample 45	C.98 Z7 12cm to 'gravel'.	C.99	Wet, fine textured. Quartz, opaque very small stones.	Spongy material with a parallel structure.	Low
Sample 49	C.104	C.105	Fine textured. Quartz, White very small stones.	Deposit similar to spongy material in sample 45.	Low
Sample 55	West boundary 50cm depth.	Negative control	Fine textured. Quartz grains. Coal type material. Small stones.	Dark organic. Conifer needle. Small roots and plant material.	No HR visible.
Sample 57	East boundary 50cm depth.	Negative control	Small stones and quartz grains.	Dried leaf and stem material. Long thin white worm (not identified).	No HR visible.

In this report we shall refer to samples using the terms in column 1 above (exhibit/item number).

VOC Analysis

Details of the sample preparation, materials and methods of analysis and results are in appendix 4.

Summary of VOC observations

The distribution of VOC hotspots is represented by the abundance of compound classes in each sample and are presented as a matrix of rows (VOC compound class) and columns (sample number) in Figure 1 which can be read with Appendix 10 as a spatial gradient across the facility sampled. For the majority of compound classes these are concentrated in samples 7, 8, 9, 14, 23, 27, 33, 46, 49 and in the Western boundary sample 55.

Individual sampling locations 1 – 49 were categorised by an osteologist as having high, medium, low or no visible densities of human remains, and this scoring is indicated in Table 2.

For some compound classes the hotspots are more widely spread across cells towards the eastern end of the alignment of cells (low sample numbers, high – medium bone density), and to a lesser extent towards the western end (high sample numbers, high – low bone density).

Of the two cells characterised as having no visible human remains, which were each sampled at several locations, one shows hotspots for most compound classes (samples 13, 14, 15; context 63) while the other only has low abundances of volatiles (samples 29, 30, 31; context 87). A third cell which was sampled at several locations also has low abundances of volatiles and low bone densities (samples 17, 18, 19; context 65).

With the exception of samples 29 – 31, cells in the central region of the cellular array are of high - medium bone density. For some of these samples abundances of volatiles are high (23, 27 and 33; context 12, 85 and 89), while for others abundances are low (21, 25, 35; context 10, 83/11 and 91).

A number of compound hotspots for different compound classes are concentrated in the Northern boundary sample rather than the Western boundary sample.

Similar compound classes, for example the various types of aldehyde, share a high degree of commonality in the location of their hotspots. However there are also examples of differentiation within a compound class according to structure and chain length (aromatic hydrocarbons; sulphur compounds DMS and DMDS; aliphatic acids).

Many of the compound classes show compound distributions consistent with known patterns of volatile emission during decomposition of mammalian tissue. These include compounds known to be produced during bone decomposition (ketones, alcohols and aldehydes). The isomer ratios for 3- and 2-methyl butanal (3-/2-) are > 1, which is a specific characteristic of human decomposition. The distribution of compound classes and of individual members within compound classes are very similar to those measured for human adult and baby positive control samples, analysed under identical conditions. There is a slightly closer similarity with the volatile profiles obtained from the human baby positive control samples.

Although all compounds detected were found in samples collected from every sampling location, there is clearly a significant concentration effect within specific cells of the cellular alignment. There does not appear to be a significant background level of volatiles of interest within those cells without distinct hotspots. The extent to which there may have been mixing and redistribution of cellular contents between cells is unknown. The concentration of volatile hotspots at specific regions within the cellular array could indicate where the highest concentration of material deposition has occurred with limited intra-cell mixing. However the apparent concentration of some of the hotspots towards the eastern and western ends of the cellular array may indicate redistribution of cellular content away from the central regions. There are hotspots within the northern and western boundary samples but not in the southern and eastern boundary samples. Whether this may represent leaching of cellular contents out of the structure is unclear and will depend on the local topography, drainage patterns and distance of the boundary sampling locations from the array.

A number of the hotspots for compounds characteristic of bone decomposition, particularly ketones, but also aliphatic alcohols and *n*-aldehydes, are found at locations with high bone densities (Table 2).

It is possible that some of the volatiles detected could have originated from the decomposition of legacy human faecal matter deposited within the cells if the structure has been used historically for treatment of human waste. For example, it is highly likely that 3- and 2-methyl butanal are present in faecal residue with the characteristic isomer ratio (Shepherd and Dawson, unpublished observations). However it is unclear whether the compounds specifically associated with decomposition of bone are similarly present in faecal residue. Limited evidence we have for soils known to be contaminated with human faeces (Shepherd and Dawson, unpublished data) suggests that these markers of bone decomposition, particularly the ketones, may indeed be present but at lower relative abundances than found in this investigation. However, there is currently insufficient experimental data regarding the persistence and characterisation of human faecal decomposition volatiles to comment further.

Figure 1. Distribution of volatiles by compound class across the cellular array.

Signature... ....Page 16 of 103

Solid organic compound analysis

Details of the sample preparation, materials and methods of analysis and results are in appendix 5.

Summary of low-volatility lipid biomarkers observations

Biomarkers compatible with human sewage (cholesterol, faecal stanols, faecal bile acids) were detected in in all analysed samples.

10-Hydroxy stearic acid, which has been used as an indicator of cadaver decomposition was also detected, but this compound has also been found to be present at relatively high concentrations in (human) sewage sludge.

The biomarker patterns (i.e. relative concentrations of individual biomarkers) were compatible with having originated from human sewage and not from farm animal waste.

The concentrations of the solid organic biomarkers in the analysed samples were much lower than would be expected if the analysed material had entirely originated from human sewage.

The two samples collected from the site boundaries had generally lower biomarker concentrations than the samples collected from within the chambers. 10-Hydroxy stearic acid, cholesterol and the faecal stanols, coprostanol and epicoprostanol have been recognised as being products of the decomposition of mammalian remains (including human), and their concentration patterns generally differ from those of human sewage material. The presence of these compounds in the samples collected from the chambers could, at least in part, have come from decomposed human bodies.

However, because of the low levels of biomarkers found in the samples from the chambers, it was not possible to assess the relative contributions from human sewage and from human body decomposition.

Total carbon and nitrogen, and stable isotope (13C and 15N) content

Details of the sample preparation, materials and methods of analysis and results are in appendix 6.

Table 3 Isotope values of the analysed samples

Context Number	Sample Number	C (%, w/w)	δ13C (‰)	N (%, w/w)	δ15N (‰)
C.51	1	18.6	-22.45	0.79	12.3
C.55	5	21.5	-23.21	0.86	11.7
C.57	7	35.7	-25.00	2.05	16.2
C.61	11	21.4	-22.63	0.88	12.3
C.63	14	12.6	-18.01	0.58	5.31
C.65	18	17.5	-22.54	0.53	5.26
C.91	35	15.9	-18.68	0.70	11.1
C.99	45	15.3	-21.56	0.71	6.14
C.105	49	25.6	-24.65	1.24	13.5
west boundary control	55	8.30	-15.16	0.33	4.44
east boundary control	57	8.82	-15.56	0.33	4.40
	bone picked out from sample 7	**13.8**	**-22.81**	2.22	10.0
Figures in bold did not contain enough material for accurate analysis.					

Sample numbers 14, 18, 45, 55 and 57 have lower carbon and nitrogen concentrations relative to the other samples collected. 14, 35, 55 and 57 also have higher C isotope ratio values, in particular the two boundary control samples (55 and 57).

10. Interpretation

Statistical analysis of the data was carried out using Primer software with square root transformation of the data (Appendix 8). The isotope plots show a clear separation of samples 55 and 57 (west boundary and east boundary locations respectively) from the other samples. Sample 14 (Context 63) is also positioned close to these two samples (no human remains observed (Table 2)). Sample 7 (context 57) which registered as a high density of human remains was furthest removed from the control boundary samples on this plot.

The sterol and stanol and the bile acids also show clear separation of samples 55 and 57. The bile acid data also shows sample 45 (Context 99) to be similar to the boundary samples. The VOC data shows less of a clear distinction between samples, possibly as a result of the mobility of these compounds and that there had been movement of water through the chambers over time The depth of the deposits from which samples were recovered were such that it is highly likely that ground water has influenced the dispersal of remains within the context (sampling submission form, page 2, Niamh McCULLAGH).

11. Conclusions

It can be confirmed from this series of analyses that there is evidence that the site *had* previously been used as a sewage facility in the past.

The results of these tests however cannot establish categorically whether the sewage facility was being used at the time when the human remains were deposited.

The results of these tests cannot establish categorically whether the non-decomposed human remains had been deposited in the chambers, or whether the bodies have previously been stored (and decomposed) elsewhere, with mainly the bones being placed in the chambers.

It does appear that the volatile organic profiles are characteristic of decomposition of mammalian tissue *or* waste, probably human. It is not possible to determine the extent to which the deposited human infant remains which are known to be present may have contributed to this, or to what extent human faecal material may also have done so. The presence of hotspots within the northern and western boundary samples but not the southern and eastern boundary samples is of note. A number of the hotspots for compounds characteristic of bone decomposition, particularly ketones, but also aliphatic alcohols and *n*-aldehydes, are found at locations with high bone densities.

The concentrations of the solid organic biomarkers in the analysed samples were very low, much lower than would be expected if the analysed material had entirely originated from human sewage waste. The samples collected from the site boundaries (samples 55, west boundary and 57, east boundary) had generally lower biomarker concentrations than the samples collected from within the chambers where remains were located. 10-Hydroxy stearic acid, cholesterol and the faecal stanols, coprostanol and epicoprostanol have been recognised as being products of the decomposition of mammalian remains (including human), and their concentration patterns generally differ from those of human sewage material. The presence of these compounds in the samples collected from the chambers could, at least in part, have come from decomposed human bodies.

The reasons for the low biomarker concentrations found in the samples are not easy to assess. If the chambers represented a closed cesspit or a number of cesspits, it is possible that the collected sewage had been removed before depositing the human cadaver material; soil may have been added at the same time, or soil may have seeped in from the roofs of the chambers. If there were one or more pipe outflows (i.e. the facility was a septic tank, or was connected to a sewer outflow), it would be expected that little sewage would be left behind).

Samples 55 and 57 (west boundary and east boundary locations respectively) and sample 14 (no visible human remains) have different isotopic profiles to the other samples examined, likely reflecting no influence from human remains or sewage.

It is likely that some analytical signature due to faecal material is present, but it is also likely that the human remains have also contributed to the analytical signatures observed, and the presence of compounds associated with decomposition of bone at locations of high bone density in the samples is suggestive of this.

Appendices

Appendix 1

Table 1 Samples received at James Hutton Institute on 15th February 2017

Case Code	MBHCOI_TM0117_	NMcC	Niamh McCullagh
GPS Location	544,066,712,178	AH	Aidan Harte
	Mother and Baby Home	LL	Linda Lynch
Client	Commission of Investigation		

Z4	Z8
Z3	Z7
Z2	Z6
Z1	Z5

N ↑

Sample number	Date	Time	Location	Context number	Collected by	Witnessed by	
001	8_2_2017	13:49	C.50.Z1: 20cm to 'gravel'	C.51	NMcC	AH, LL	
002	8_2_2017	13:49	C.50.Z1: Control of 001	C.51	NMcC	AH, LL	RETAINED
003	8_2_2017	14:04	C.52.Z6: 15cm to 'gravel'	C.53	NMcC	AH, LL	
004	8_2_2017	14:04	C.52.Z6: Control of 003	C.53	NMcC	AH, LL	RETAINED
005	8_2_2017	14:19	C.54.Z6: 25cm to 'gravel'	C.55	NMcC	AH, LL	
006	8_2_2017	14:19	C.54.Z6: Control of 005	C.55	NMcC	AH, LL	RETAINED
007	8_2_2017	14:38	C.56.Z1	C.57	NMcC	AH, LL	
008	8_2_2017	14:38	C.56.Z1: Control of 007	C.57	NMcC	AH, LL	RETAINED
009	8_2_2017	14:50	C.58.Z7: 30cm to 'gravel'	C.59	NMcC	AH, LL	
010	8_2_2017	14:50	C.58.Z7: Control of 009	C.59	NMcC	AH, LL	RETAINED
011	8_2_2017	16:37	C.40.Z6: 12cm to 'gravel'	C.41	NMcC	AH, LL	
012	8_2_2017	16:37	C.40.Z6: Control of 011	C.41	NMcC	AH, LL	RETAINED
013	8_2_2017	16:48	C.42.Z6: No HR visible 4cm to 'gravel'	C.43	NMcC	AH, LL	
014	8_2_2017	16:49	C.42.Z7: No HR visible 4cm to 'gravel'	C.43	NMcC	AH, LL	
015	8_2_2017	16:49	C.42.Z1: No HR visible 2cm to 'gravel'	C.43	NMcC	AH, LL	
016	8_2_2017	16:53	C.42.Z8: Control of 013-015	C.43	NMcC	AH, LL	RETAINED
017	8_2_2017	16:59	C.64.Z6: No HR visible 11cm to 'gravel'	C.65	NMcC	AH, LL	
018	8_2_2017	17:00	C.64.Z7: No HR visible 14cm to 'gravel'	C.65	NMcC	AH, LL	
019	8_2_2017	17:02	C.64.Z2: No HR visible 12cm to 'gravel'	C.65	NMcC	AH, LL	
020	8_2_2017	17:04	C.64.Z5: Control of 017-019	C.65	NMcC	AH, LL	RETAINED
021	8_2_2017	17:04	C.102.Z8: 20cm to 'gravel'	C.10	NMcC	AH, LL	
022	8_2_2017	17:04	C.102.Z8: Control of 021	C.10	NMcC	AH, LL	RETAINED
023	8_2_2017	17:25	C.102.Z7: 25cm to 'gravel'	C.12	NMcC	AH, LL	
024	8_2_2017	17:25	C.102.Z7: Control of 023	C.12	NMcC	AH, LL	RETAINED
025	8_2_2017	17:33	C.11/82.Z8: 30cm to 'gravel'	C.83/11	NMcC	AH, LL	
026	8_2_2017	17:33	C.11/82.Z8: Control of 025	C.83/11	NMcC	AH, LL	RETAINED
027	8_2_2017	17:40	C.84.Z2: 21cm to 'gravel'	C.85	NMcC	AH, LL	
028	8_2_2017	17:40	C.84.Z2: Control of 027	C.85	NMcC	AH, LL	RETAINED
029	8_2_2017	16:49	C.86.Z4: 14cm to 'gravel'	C.87	NMcC	AH, LL	
030	8_2_2017	17:50	C.86.Z7: 21cm to 'gravel'	C.87	NMcC	AH, LL	
031	8_2_2017	17:52	C.86.Z2: 25cm to 'gravel'	C.87	NMcC	AH, LL	
032	8_2_2017	17:55	C.86.Z5: Control of 029-031	C.87	NMcC	AH, LL	RETAINED
033	8_2_2017	18:01	C.88.Z6: 5cm to resistance	C.89	NMcC	AH, LL	
034	8_2_2017	18:01	C.88.Z6: Control of 033	C.89	NMcC	AH, LL	RETAINED
035	8_2_2017	18:08	C.90.Z5: 15cm to 'gravel' includes bone	C.91	NMcC	AH, LL	
036	8_2_2017	18:08	C.90.Z7: Control of 035	C.91	NMcC	AH, LL	RETAINED
037	8_2_2017	18:11	C.92.Z7: 21cm to 'gravel'	C.93	NMcC	AH, LL	
038	8_2_2017	18:11	C.92.Z7: Control of 037	C.93	NMcC	AH, LL	RETAINED
039	9_2_2017	10:46	C.94.Z1 15cm to 'gravel'	C.95	NMcC	AH, LL	
040	9_2_2017	10:48	C.94.Z1 Control to 039	C.95	NMcC	AH, LL	RETAINED
041	9_2_2017	10:48	C.92 Atmospheric inside chamber		NMcC	AH, LL	
042	9_2_2017	10:48	C.92 Atmospheric inside chamber Control		NMcC	AH, LL	RETAINED
043	9_2_2017	10:54	C.96.Z6 25cm to 'gravel'	C.97	NMcC	AH, LL	
044	9_2_2017	10:54	C.96.Z6 Control to 043	C.97	NMcC	AH, LL	RETAINED
045	9_2_2017	11:00	C.98.Z7: 12cm to 'gravel'	C.99	NMcC	AH, LL	
046	9_2_2017	11:00	C.98.Z7: Control to 045	C.99	NMcC	AH, LL	RETAINED
047	9_2_2017	11:06	C.100.Z8 15cm to 'gravel'	C.101	NMcC	AH, LL	
048	9_2_2017	11:06	C.100.Z8: Control to 047	C.101	NMcC	AH, LL	RETAINED
049	9_2_2017	11:23	C.104	C.105	NMcC	AH, LL	
050	9_2_2017	11:23	C.104 Control	C.105	NMcC	AH, LL	RETAINED
051	9_2_2017	11:21	Baulk in T6	C.2	NMcC	AH, LL	
052	9_2_2017	11:21	Baulk in T6 Control	C.2	NMcC	AH, LL	RETAINED
053	9_2_2017	11:27	North boundary 60cm depth		NMcC	AH, LL	
054	9_2_2017	11:27	North boundary 60cm depth Control		NMcC	AH, LL	RETAINED
055	9_2_2017	11:30	West boundary 50cm depth		NMcC	AH, LL	
056	9_2_2017	11:30	West boundary 50cm depth Control		NMcC	AH, LL	RETAINED
057	9_2_2017	11:33	East boundary 50cm depth		NMcC	AH, LL	
058	9_2_2017	11:33	East boundary 50cm depth Control		NMcC	AH, LL	RETAINED
059	9_2_2017	11:35	South boundary 50cm depth		NMcC	AH, LL	
060	9_2_2017	11:35	South boundary 50cm depth Control		NMcC	AH, LL	RETAINED
061	9_2_2017	12:30	Atmospheric outside tank		NMcC	AH, LL	
062	9_2_2017	12:30	Atmospheric outside tank Control		NMcC	AH, LL	RETAINED
063	9_2_2017	NA	Blank unopened type I		NMcC	AH, LL	
064	9_2_2017	NA	Blank unopened type I Control		NMcC	AH, LL	RETAINED

Signature... Lorna Dawson ....Page 22 of 103

065	9_2_2017	NA	Blank unopened type II	NMcC	AH_11	
066	9_2_2017	NA	Blank unopened type II Control	NMcC	AH_11	RETAINED

Signature... ....Page 23 of 103

Appendix 2

Audit Trail

MBHCOI_TM0117_					
NOTE: All sample examination, description and preparation for analysis carried out in secure lab 234.					
Date	Analyst	Sample ID	Method	Type	Hutton ID
15/02/2017			Samples received from DHL Couriers. One large box containing 2 sealed evidence bags		
15/02/2017	L. Dawson, J. Ross		The bags were opened, samples checked, then bags resealed.		
16/02/2017	L. Dawson		Samples taken to Tom Shepherd at Dundee site who signed a record of receipt.		
06/04/2017	H. Watson, C. Taylor		Samples brought back to Aberdeen in sealed container.		
17/04/2017	L. Dawson, J. Ross	1, 5, 7, 11, 14, 18, 35, 45, 49, 55, 57	These samples were chosen for biomarker analysis		
17/04/2017	L. Dawson, J. Ross	1	The sample pot was opened, a sub-sample taken to a petri dish, described and placed in an oven @ 40 degrees C overnight.	Soil	
17/04/2017	L. Dawson, J. Ross	5	The sample pot was opened, a sub-sample taken to a petri dish, described and placed in an oven @ 40 degrees C overnight.	Soil	
17/04/2017	L. Dawson, J. Ross	7	The sample pot was opened, a sub-sample taken to a petri dish, described and placed in an oven @ 40 degrees C overnight.	Soil	

Signature... Lorna Dawson

17/04/2017	L. Dawson, J. Ross	11	The sample pot was opened, a sub-sample taken to a petri dish, described, crystallized material was taken to a vial labelled LD1, then the vial and sub-sample placed in an oven @ 40 degrees C overnight.	Soil LD1 crystallized material	
17/04/2017	L. Dawson, J. Ross	14	The sample pot was opened, a sub-sample taken to a petri dish, described and placed in an oven @ 40 degrees C overnight.	Soil	
17/04/2017	L. Dawson, J. Ross	18	The sample pot was opened, a sub-sample taken to a petri dish, described and placed in an oven @ 40 degrees C overnight.	Soil	
17/04/2017	L. Dawson, J. Ross	35	The sample pot was opened, a sub-sample taken to a petri dish, described,a flake of material (query bone) was taken to a vial labelled LD2, then the vial and sub-sample placed in an oven @ 40 degrees C overnight.	Soil LD2 possible bone	
17/04/2017	L. Dawson, J. Ross	45	The sample pot was opened, a sub-sample taken to a petri dish, described and placed in an oven @ 40 degrees C overnight.	Soil	
17/04/2017	L. Dawson, J. Ross	49	The sample pot was opened, a sub-sample taken to a petri dish, described and placed in an oven @ 40 degrees C overnight.	Soil	
17/04/2017	L. Dawson, J. Ross	55	The sample pot was opened, a sub-sample taken to a petri dish, described and placed in an oven @ 40 degrees C overnight.	Soil	
17/04/2017	L. Dawson, J. Ross	57	The sample pot was opened, a sub-sample taken to a petri dish, described and placed in an oven @ 40 degrees C overnight.	Soil	
18/04/2017	L. Dawson, J. Ross	1	Sample given a Hutton ID code, photographed, hand ground and weighed for biomarker analysis.		1259284

Signature... ....

18/04/2017	L. Dawson, J. Ross	5	Sample given a Hutton ID code, photographed and pieces of material which could be bone picked out to a petri dish. The sample was then hand ground and weighed for biomarker analysis.		1259285
18/04/2017	L. Dawson, J. Ross	7	Sample photographed and pieces of material which could be bone picked out to a petri dish. The sample was then hand ground and weighed for biomarker analysis.		1259286
18/04/2017	L. Dawson, J. Ross	11	Sample given a Hutton ID code, photographed, hand ground and weighed for biomarker analysis.		1259287
18/04/2017	L. Dawson, J. Ross	14	Sample given a Hutton ID code, photographed, hand ground and weighed for biomarker analysis.		1259288
18/04/2017	L. Dawson, J. Ross	18	Sample given a Hutton ID code, photographed, hand ground and weighed for biomarker analysis.		1259289
18/04/2017	L. Dawson, J. Ross	35	Sample given a Hutton ID code, photographed and pieces of material which could be bone picked out to a petri dish. The sample was then hand ground and weighed for biomarker analysis.		1259290
18/04/2017	L. Dawson, J. Ross	45	Sample given a Hutton ID code, photographed, hand ground and weighed for biomarker analysis.		1259291
18/04/2017	L. Dawson, J. Ross	49	Sample given a Hutton ID code, photographed, hand ground and weighed for biomarker analysis.		1259292
18/04/2017	L. Dawson, J. Ross	55	Sample given a Hutton ID code, photographed, hand ground and weighed for biomarker analysis.		1259293

Signature... Lorna Dawson

18/04/2017	L. Dawson, J. Ross	57	Sample given a Hutton ID code, photographed, hand ground and weighed for biomarker analysis.		1259294
19/04/2017	L. Dawson, J. Ross	7	A small piece of the material which could be bone was hand ground and given a Hutton ID code.		1259295
19/04/2017	J. Ross, G Martin		Samples 1259284-1259295 were given to Gillian Martin for 13C and 15N analysis.		
21/04/2017	J. Ross, G Martin		Samples 1259284-1259295 were returned to lab 234 by Gillian Martin.		

Signature... ....Page 27 of 103

Appendix 3

References

Cognat C., Shepherd, T., Verrall S. R. & Stewart, D. 2012. Comparison of two headspace sampling techniques for the analysis of off-flavour volatiles from oat based products. Food Chemistry. 134, 1592-1600.

Dawson, L.A. and Hillier, S. (2010) Measurement of soil characteristics for forensic applications. Surface and Interface Analysis. 42, 363-377.

Dawson, LA. and Mayes, RW. (2014) Criminal and Environmental Soil Forensics, In: B Murphy & R Morrison (eds), Introduction to Environmental Forensics, 3rd Edition. Academic Press.

Deasy, W., Shepherd, T., Alexander, C. J., Birch A. N. E. and Evans K. A. 2016a. Development and validation of a SPME-GC-MS method for in situ passive sampling of root volatiles from glasshouse-grown broccoli plants undergoing below-ground herbivory by larvae of cabbage root fly, Delia radicum L. Phytochemical Analysis, 27, 375-393.

Deasy, W., Shepherd, T., Alexander, C. J., Birch A. N. E. and Evans K. A. 2016b. Field-based evaluation of a novel SPME-GC-MS method for investigation below ground interaction between brassica roots and larvae of cabbage root fly, Delia radicum L. Phytochemical Analysis, 27, 343-353.

Decreux, L. G.. M., Morris, W. L., Prosser, I. M., Morris, J. A., Beale, M. A., Wright, F., Shepherd, T., Bryan, G. J., Hedley, P. E. & Taylor, M. A. 2008. Expression profiling of potato germplasm differentiated in quality traits leads to the identification of candidate flavour and texture genes. Journal of Experimental Botany 59, 4219-4231.

McMenemy, L.S., Hartley, S.E., MacFarlane, S.A., Karley, A.J., Shepherd, T. & Johnson, S.N. 2012. Raspberry viruses manipulate the behaviour of their insect vectors. Entomologia Experimentalis et Applicata, 144, 56-68.

Morris, W. L., Shepherd, T., Verrall, S. R., McNicol, J.W. & Taylor, M. A. 2010. Relationships between volatile and non-volatile metabolites and attributes of processed potato flavour. Phytochemistry, 71, 1765-1773.

Thornton et al, (2015) Distributions of carbon and nitrogen isotopes in Scotland's topsoil: a national-scale study. European Journal of Soil Science. 66, 1002-1011.

Vaas, A.A., Smith, R.R., Thompson, C. V., Burnett, M.N., Wolf, D. A., Synstelien, J.A., Dulgerian, N. and Eckenrode, B. 2004. Decompositional odor database. Journal of Forensic Science, 49, 1-10.

Vaas, A.A., Smith, R.R., Thompson, C. V., Burnett, M.N., Dulgerian, N. and Eckenrode, B. 2008. Odor analysis of decomposing buried human remains. Journal of Forensic Science, 53, 384-391.

Vaas, A.A. 2012. Odor mortis. Forensic Science International 222, 234-241.

Appendix 4

VOC analysis

Solid Phase Microextraction (SPME)

In the SPME technique, a short (1 cm) fibre coated with a thin film of polymeric adsorbant is exposed in the headspace above the sample, which is sealed in a glass vial and heated within a temperature controlled incubator. During the exposure period volatiles released from the sample are entrained and concentrated *in-situ* within the fibre film. After a defined period, the fibre is withdrawn into a protective sheath and removed from the sample vial. The fibre is subsequently re-exposed within the injector of a GC-MS instrument, and the entrained volatiles are desorbed directly into the gas chromatography column, where they are separated into individual constituents and passed to the mass spectrometer for characterisation and identification. The methodology used was based on SPME techniques developed in our laboratories for analysis of cooked potato flavour volatiles (Decreux et al., 2008), for analysis of plant leaf derived volatiles (McMenemy et al., 2012) and for analysis of plant root-derived volatiles collected in situ (Deasy et al., 2016a, b).

GC -MS

During the gas chromatographic phase of the analysis, analytes are separated by passage through the GC column, a long length of narrow bore silica glass tubing, the inside of which is coated in very thin layer of a polymeric material, the stationary phase. The complex mixture of analytes is carried onto one end of the GC column by a flow of inert helium gas which flows continuously through the column. Individual analytes interact differentially with the stationary phase, migrating along the column at different rates. In addition, the GC column, which is located within a temperature controlled oven, is heated at a predetermined rate to accelerate analyte migration. Analytes then pass from the GC into the mass spectrometer via a heated transfer line, where they undergo mass spectrometric analysis.

During mass spectral analysis, analytes under high vacuum are ionized by high energy electrons with a set energy of 70eV. An electron is knocked out from the electronic structure of the analyte, to form ions carrying a single positive charge (electron ionization EI). Each ion formed has a specific mass to charge ratio (*m/z*) which is effectively the mass of the ion since the charge is unity. The initial product of ionization is an ionized intact molecule, the molecular ion (M). However the EI process transfers a lot of excess energy to the molecular ion, which is lost or redistributed by the break-up (fragmentation) of the ion. Depending on the structure of the ion (and hence of the intact analyte), a whole range of fragments with different atomic compositions and different masses (*m/z*) are generated, and in turn some of the fragment ions will themselves fragment further. At the end of the process, each analyte generates a range of fragment ions, often including some intact molecular ions, each of which has a relative abundance unique to the analyte. This is the mass spectrum which is usually depicted graphically as a series of vertical lines showing ions of increasing mass (x-axis) against their abundance (z-axis). Use of EI at 70 eV is an accepted international standard, and all GC-MS systems are generally operated in this way. Consequently, MS analyses of the same analytes will generate broadly similar mass spectra Irrespective of instrument manufacturer, location or operator. This has led to compilation of large databases of EI (70 eV) mass spectra which can be searched using computerized data systems to aid in the identification of analytes.

The mass spectrometer analyses the content of the GC effluent as it passes into the instrument by sampling the ions present over a pre-set mass range (one scan, 30-400 amu) repeatedly and rapidly (6 scans/sec) for the duration of the analysis. One scan constitutes a single mass spectrum, and 6 mass spectra are generated each second. Each mass spectrum incorporates abundance data for each ion detected. If the ion abundances for all ions in a scan are summed and then are displayed for separate scans along a time (x) axis against abundance (y axis), a chromatographic trace is generated, the Total Ion Chromatogram (TIC).

Individual compounds have a compound-specific mass spectrum which is often unique to the compound or has unique compound class-related characteristics. In addition individual compounds generally have a unique retention time on chromatographic separation by GC. Both of these attributes are used to characterize each compound. However, for a complex mixture of compounds, it is usually the case that not all of the individual components present will be chromatographically resolved in the TIC traces, ie there will be overlap to various degrees with different compounds co-eluting. The mass spectra of individual co-eluting compounds usually contain some ions or ion groups, with different masses which are unique to each compound in the mixture and are not common to the other compounds present. This property is used In order to de-convolute overlapping and co-eluting peaks. Using the software packages such as Xcalibur™, selected ion chromatograms (SIC) for these ions unique to each component can be extracted from the raw data. SIC traces show how the abundance of the chosen ion(s) change with time, and overlapping and co-eluting peaks can usually be resolved into their individual constituents. A measure of the abundance of the compounds present is made by integrating the SIC traces.

Materials and Methods

Sample preparation

Sample numbers were inscribed onto the side of clean, empty 20 mL screw top headspace vials (Supelco, UK) using an indelible marker pen, and the vials were flushed out with dry filtered nitrogen at > 500 mL/minute for 30 seconds and then capped. The vials were weighed and placed in the fume cupboard prior to transfer of soil samples.

Soil samples were allowed to warm to room temperature, then the large sample vial and weighed headspace vial were both opened, and a subsample of soil was transferred to the weighed vial using a clean spatula until it was approximately 1/4 to 1/3 full. Care was taken to ensure there was no sample adhering to the neck of the vial which would interfere with insertion of the SPME fibre assembly through the vial cap septum. Both vials were capped and sealed. The weighed vial containing the transferred sample was reweighed and then transferred to a cold room at -20°C for storage overnight.

Individual samples were loaded onto a CombiPal autosampler (CTC Analytics, Switzerland) for automated sampling using solid phase micro extraction (SPME) for trapping of volatiles and analysis by gas chromatography-mass spectrometry (GC-MS). A sample blank containing a mixture of laboratory and fume cupboard air was prepared by leaving an empty uncapped vial exposed within the fume cupboard for 5 minutes before the vial was capped. A sampling schedule for preparation and analysis of all samples is shown in Appendix 1, Table 1.

Analysis of soil volatiles by SPME-GC-MS

Samples were analysed using a Trace DSQII GC-MS (Thermo Scientific, Hemel Hempstead, U.K.) fitted with a CombiPal autosampler configured for use with SPME fibers. Volatiles were trapped using a polydimethylsiloxane/divinylbenzene (PDMS/DVB) SPME fibre (23 gauge, 65mm film, Supelco, UK) at 75°C for 30 minutes. During entrainment the vial was maintained at the appropriate temperature in a heated incubator which formed part of the autosampler assembly. Volatiles were desorbed from the SPME fibre isothermally at 250°C for 2 minutes within a programmable temperature vapourising (PTV) injector operating in splitless mode and fitted with a Merlin Microseal™ high pressure septum (Agilent Technologies, UK). Compounds were separated on a DB 1701 GC column (30m x 0.25 mm i.d x 0.25 μm, Agilent Technologies, UK) using helium at 1.5 mL/min in constant flow mode. The GC oven temperature was held for 2.0 min at 40°C followed by a 10°C/min temperature increase up to 240°C with a further 10 minute isothermal hold at that temperature. The GC-MS interface temperature was 250°C and the MS was used in electron ionisation (EI) mode at 70 eV over a mass range of 25-400 amu with a source temperature of 200°C. Data was acquired at 6 scans/sec and analysed using the Xcalibur™ software package V. 2.07 (ThermoFisher, UK). Immediately following the desorbtion of volatiles from the fibre into the PTV injector, the fibre was automatically reconditioned at 250°C for 30 minutes, under a flow of dry nitrogen, using a reconditioning station attachment for the GC-MS autosampler. At the end of this time, and following a short period for re-equlibration of the GC, the instrumentation was ready for loading and analysis of the next soil sample.

The sample methodology normally ensures that the same individual SPME fibre was used for entrainment and analysis of each sample. However, during the course of the analysis two separate fibres from the same manufacturing batch were used. Fibre 2 was used for trapping volatiles from a laboratory control air blank and samples 001 - 013 and 049 – 059. Fibre 3 was used for samples 013 – 047.

VOC results

Although an attempt was made to ensure that the samples from which volatiles were trapped were visually of a similar size by volume, sample weights ranged from 0.971 - 4.205 g probably due to variation in moisture content, particle size and density. Initially, abundance data was generated as total abundance of each compound per sample, from which the abundance per gram of sample was calculated. The proportional abundance for each analyte in each sample taken from individual cells (samples 001 – 049) was calculated as a percentage of the combined total abundance of the analyte for all these cells. Proportional abundances for compounds in the Baulk sample (051) and in the north, west, east and south boundary samples (053, 055, 057, 059) were also calculated relative to their combined total abundance for samples 001 – 049. The data in Appendix 2, Table 3, ordered according to analyte class, is presented both as abundance per gram of sample and as the proportional abundances of individual compounds in each sample (sum for samples 001 – 049 = 100). In addition, for each analyte class, these two abundance values for constituent compounds are also plotted graphically in sample order in order to provide a means of visualizing their spatial distribution.

Among the structural analyte classes present, most are aliphatic compounds consisting of chains of methylene units (CH_2) with various attached functional groups and substituents which define the compound class. Some compound classes consist of ring structures, incorporating benzene (aromatic compounds) or furan, to which functional groups and other substituents may be attached. Eleven groupings are defined:

(1) Aliphatic alcohols, aromatic alcohols and phenol; (2) Sulfur compounds; (3) Ketones; (4) Halocarbons (halogenated compounds); (5) Furans; (6) Branched chain (*br*-) aldehydes and aromatic aldehydes; (7) Saturated straight chain (*n*-) aldehydes; (8) Aromatic hydrocarbons (benzene derivatives and pyridine); (9) Carboxylic acids; (10) Unsaturated *n*-aldehydes; (11) Alkanes (aliphatic *n*- saturated hydrocarbons)

All listed compounds were found to be present in virtually all samples at varying abundances, and at abundances considerably greater than measured in laboratory air controls (data not shown in tables). A single sample was taken from most cells; however there were three instances where three samples were taken from the same cell. These are highlighted by yellow, green and blue colour bands in Appendix 2, Table 3, . Of these there was no visible evidence of human remains in two of the groupings (samples 013, 014, 015, yellow background; samples 029, 030, 031, blue background). The baulk sample (051) is highlighted pink and the four boundary samples (053, 055, 057 and 059) in grey. The same colour scheme is used to delineate the location of the same sample groups in the accompanying graphical plots. In the following interpretation of the results both measurements of abundance were used in combination to assess if compounds were present at a particular location at significantly elevated levels.

Interpretation of the data was based on comparison of the distribution of the volatile compounds found in the samples with published data describing the range of volatile compounds produced during decomposition of mammalian tissues, including that of humans (Vaas et al., 2004, 2008; Vaas, 2012). The use of VOC analysis in this way to characterize the odour of decomposition is relatively recent and is considered an experimental technique still under development. The data compiled by Vass was largely based on use of polymer entrainment techniques for recovery of volatiles from burials within body farms within the USA. Use of SPME for trapping of volatiles is a recent modification of the polymer entrainment methods, and lacks the equivalent range of positive control data. However we have recently analysed the volatile profiles from two positive control samples (soil from the grave of an adult female buried for 15 years and residue (possibly adipocere) from the burial of a full term baby for 6 months) under identical conditions as used in this investigation (Shepherd and Dawson, unpublished data). This data is also used for comparison with that generated in this investigation.

Aliphatic alcohols, aromatic alcohols and phenol

The aliphatic alcohols ethanol (C_2), 1-pentanol (C_5), 1-hexanol (C_6), 1-heptanol (C_7) and the aromatic compound phenol are known non-specific markers of bone decomposition in mammals. Although not usually a major product of decomposition in humans, they may be significant in decomposition of other animals such as dogs or pigs (Vaas et al., 2004, 2008; Vaas, 2012). Ethanol, 1-pentanol, 1-heptanol, 1-octanol (C_8), 1-octen-3-ol (C_8) were present in the positive human control SPME samples in the abundance order octanol > heptanol > pentanol > ethanol along with the aromatic alcohol phenylmethanol and phenol (Shepherd and Dawson, unpublished data). Ethanol, hexanol, heptanol, octanol, 1-octen-3-ol phenylmethanol and phenol were found in the samples.

In terms of abundance per g of sample and proportional abundance, hotspots are found for phenol and phenylmethanol in samples 7 – 15, 23, 33, and 39-45. Collectively for ethanol, 1-hexanol and 1-heptanol, hotspots are found for samples 7, 9, 11, 23, 27, 33, 45 and 49. Hotspots for 1-octanol and 1-octen-3-ol were found for samples 7-15, 23, 45 and 49.

High abundances of these compounds, particularly phenyl methanol and the C_8 alcohols were also found for the West boundary control sample (55).

Abundances of these compounds were low in one of the cells with no visible human remains (samples 29 – 31), but showed a peak for some components in the other (samples 13 – 15).

Sulfur compounds

Sulfur compounds, including carbon disulfide, carbon oxide sulfide (COS), dimethyl sulfide (DMS), dimethyl disulfide (DMDS), dimethyl trisulfide, and dimethyl tetrasulfide (DMTS) are non-specific markers of mammalian decomposition (Vaas et al., 2004, 2008; Vaas, 2012). DMS, DMDS and

DMTS may be associated with late, mid and early stages of decomposition respectively. In the SPME positive controls, DMS was only detected in the adult control samples, whereas DMDS and DMTS were only detected in the baby control (DMTS > DMDS), consistent with decomposition stage differences as described by Vaas (Shepherd and Dawson, unpublished data).
Only dimethylsulfide and dimethyldisulfide were detected in the samples.

Proportional abundance and abundance per g for DMS is fairly uniform across the samples with perhaps an indication of an increase for cells located towards the west (higher sample number). The abundance for this compound is significantly greater for the West boundary control sample (55). The abundance profiles for DMDS show maxima for samples 11-14, the west tending samples 27-49, the Baulk sample (51) and to a lesser extent North boundary control (53). The abundances of DMDS in the other boundary samples, including the West boundary sample (55) are relatively low in comparison.

Ketones

Several ketones have been associated with human and other mammalian decomposition, particularly of bone, and these include acetone (2-propanone), 2-butanone (methyl ethyl ketone, MEK), 2-nonanone and 2-decanone (Vaas et al., 2004, 2008; Vaas, 2012). In all these compounds the carbonyl functional group is located at C-2 of the carbon chain. There were high abundances of ketones in the range C_3-C_{15} in the SPME positive control baby residue and adult soil samples, with the chain length distribution peaking at 2-Decanone (C_{10}) (Shepherd and Dawson, unpublished data).
Thirteen ketones of this type were detected in the samples of increasing size from C_3 up to C_{13}. These include 2-propanone (acetone, C_3), 2-pentanone (C_5), 2-hexanone (C_6), 2-heptanone (C_7), 2-octanone (C_8), 2-nonanone (C_9), 2-decanone (C_{10}), 2-undecanone (C_{11}), 2-dodecanone (C_{12}) and 2-tridecanone (C_{13}). In addition the branched saturated and unsaturated C_8 homologues of this series, 6-methyl-2-heptanone and 6-methyl-5-hepten-2-one, were also found along with the C_8 compound 3-octanone, which has the keto group at C-3. A C_4 diketo compound, 2,3-butanedione and an aromatic ketone acetophenone were also present.
Abundance hotspots for the C-2 ketones were found for samples 1-11, 23, 27, 33, 45 and 49, particularly for the 2-decanone (C_{10}), 2-undecanone (C_{11}), and to a lesser extent for 2-pentanone (C_5) 2-octanone (C_8) and 2-nonanone (C_9). Higher levels of the C-3 ketone 3-octanone (C_8) were associated with samples 23 and 45.
The western control also showed appreciable abundances of some of these compounds, particularly 2-hexanone (C_6) and the branched C_8 compounds 6-methyl-2-heptanone and 6-methyl-5-hepten-2-one.
Ketones were generally of lower abundance in one of the samples from cells with no visible human remains (29-31), but were of higher abundance for some components in the other (samples 13 – 15).

Halocarbons

A number of halogenated compounds such as chloroform, carbon tetrachloride, di- or trichloroethylene and various chloro-fluorocarbons are associated with mammalian decomposition (Vaas et al., 2004, 2008; Vaas, 2012). Of these, carbon tetrachloride has been identified as a specific marker of human decomposition, produced during the early phase of decomposition. Chlorofluorocarbons are not expected to be found for children under 4 years old, and would also not be expected for any burials in the period prior to the fluoridation of water. Chloroform and dichloromethane (DCM) were found in the positive SPME controls (chloroform > DCM), however carbon tetrachloride was not detected (Shepherd and Dawson, unpublished data).
Detailed examination of the data failed to show any evidence for the presence of carbon tetrachloride or chlorofluorocarbons, and dichloromethane and chloroform were the only halocarbons detected in the samples.

Abundance profiles for dichloromethane and chloroform were broadly similar across the samples, with abundance maxima for samples 7, 9 and an increase towards the western cells (higher sample numbers) and baulk sample (51) culminating with maximum abundance for the Northern boundary sample (53).

Furans

Furans, including 2-methyl furan and furans with other substituents, are found in adult human and animal decomposition, but may not be expected (2-methyl furan) for children under 4 years old (Vaas et al., 2004, 2008; Vaas, 2012). Most of these components, in particular furfural and 2-pentyl furan, were present in the SPME positive control samples (Shepherd and Dawson, unpublished data).
A series of four alkyl substituted furans was found in the samples. Most of the compounds present were substituted at C-2 in the furan ring (2-methyl-, 2-ethyl- and 2-pentylfuran) and one at C-3 (3-methylfuran). Reduced (hydrogenated) furan derivatives, 2,3-dihydrofuran and tetrahydrofuran (THF) were also detected along with the aldehyde furfural (furan-2-carboxaldehyde).
The most abundant furan derivatives were 2-pentyl furan with hotspots at samples 1-7, 11, 23, 27, 49 and the western boundary sample (55) and THF with hotspots at samples 1-15, 33-45, 49, baulk sample 51 and the Northern (53) and Western boundary samples (55). The distribution of the other furans follows a broadly similar pattern to a combination of those for 2-pentylfuran and tetrahydrofuran.

Branched chain (br-) aldehydes and aromatic aldehydes

Branched (*br*-) short chain aldehydes 2-methyl propanal, 3-methyl butanal and 2-methyl butanal are considered to be key indicators of mammalian decomposition. The ratio of 3-methyl butanal to 2-methyl butanal (3-/2-) is considered a key factor distinguishing human remains from those of other animals. A greater abundance of the 3- isomer relative to the 2- isomer (ratio of 3-/2- > 1) being indicative of human decomposition, whereas for other mammals, the 2- isomer is more abundant (ratio of 3-/2- < 1) (Vaas, 2012). These aldehydes were present in the SPME positive control samples, and the methylbutanal isomer ratios (3-/2-) were 2.6-3.3 for the adult control and 7.0 for the baby control (Shepherd and Dawson, unpublished data).

The three short chain branched aldehydes, 2-methylpropanal, 3-methylbutanal and 2-methyl butanal were detected in all samples with 3-/2- isomer ratios in the range of 1.27 – 3.07 for all but one sample (5) which had an isomer ratio 1.01. These isomer ratios are consistent with a human decomposition process.

The *br*-aldehydes were most abundant for samples 5, 7, 11, 14, 45 and 49, and for the Western boundary sample (55).

The presence of the benzenoid aldehyde benzaldehyde and the related compound phenylacetaldehyde may be associated with decomposition (Vaas et al., 2004, 2008; Vaas, 2012). Both were present in the SPME positive control samples (benzaldehyde > phenylacetaldehyde)

Benzaldehyde and phenylacetaldehyde were found in the samples, with broadly similar abundance profiles. Abundance maxima were seen for samples 1-9, 11-15, 23, 27, 33, 49, and for the Western boundary sample (55).

***n*-Aldehydes**

Straight chain aldehydes in the range C_5 to C_{11} are among the interesting marker compounds associated with mammalian and in particular bone decomposition. Increased abundance of the longer homologues is associated with the later stages of decomposition. Of these nonanal (C_9) and decanal (C_{10}) are considered of significance for burial decomposition (Vaas et al., 2004, 2008; Vaas, 2012). Aldehydes in the range C_5 to C_{11} and C_{15} were found in the SPME positive control adult and baby samples with similar chain length distributions ($C_9 > C_8 = C_{10} = C_7$) (Shepherd and Dawson, unpublished data).

Ten aldehydes of this type were detected in the samples including butanal (C_4), pentanal (C_5), hexanal (C_6), heptanal (C_7), octanal (C_8), nonanal (C_9), decanal (C_{10}), undecanal (C_{11}), dodecanal (C_{12}) and pentadecanal (C_{15}).

Of these the C_8-C_{11} aldehydes, octanal, nonanal, decanal, and unecanal were the most abundant homologues with abundance maxima for samples 1-15, 23, 27, 33, 45 and 49, and for the Western boundary sample (55).

Aromatic hydrocarbons

Several aromatic hydrocarbons including benzene, toluene (methyl benzene), isomers of dimethyl benzene (xylenes), ethyl methyl benzene and styrene (ethenyl benzene) are associated with mammalian decomposition but are considered to be non-specific. Most of the aromatic compounds are produced during all phases of decomposition, although the more substituted forms and styrene may be more prevalent in the earlier stages (Vaas et al., 2004, 2008; Vaas, 2012). These compounds were also found extensively in the SPME positive control adult and baby samples (Shepherd and Dawson, unpublished data). The aromatic nitrogen heterocycle, pyridine, was found in the SPME positive baby control, but not in the adult control (Shepherd and Dawson, unpublished data).

Eleven members of this class of compound, including benzene, toluene, ethyl benzene, ethylmethyl benzene, styrene, dimethyl styrene (or ethyl styrene), and multiple isomers of dimethyl benzene and methylisopropy benzene (or diethyl benzene) were detected in the samples. In addition the aromatic nitrogen-containing heterocyclic compound pyridine was detected.

Abundance maxima for aromatic compounds were seen for samples 5, 7, 11, 13, 13, 27, 39 - 45 and 49, and for the Northern boundary sample (53). Interestingly, there is a shift in the dominant aromatics present in the samples when moving from eastern to western cells (low to high sample numbers). The methylisopropylbenzenes and one of the dimethylbenzenes (or ethylbenzene) dominate the distribution for samples 5 and 7, whereas the methylethyl/ethymethyl benzenes dominate for samples 11, 13, 23 and 27. Styrene and ethylbenzene (or dimethylbenzene) dominate at sample 43 and toluene and ethylbenzene (or dimethylbenzene) dominate at sample 49. The dimethylbenzenes/ethylbenzene and toluene dominate in the Northern boundary sample (53). Pyridine shows abundance maxima at samples 23, 27, 37-49 and the Western boundary sample (55).

Carboxylic acids

The methyl ester of hexadecanoic acid (C_{16}) is associated with early stage decomposition (Vaas et al., 2004, 2008; Vaas, 2012). Free hexadecanoic (C_{16}) and the unsaturated hexadecenoic (C_{16}) acids were detected in the SPME positive control baby sample but not the adult samples. Shorter chain acids in the range C_2 - C_9 were detected in the positive control samples with much higher abundances for the baby control. The homolog distributions were also different for the baby ($C_9 > C_8 > C_6 > C_7 = C_2 > C_3 > C_4 = C_5$) and adult ($C_8 > C_2 > C_6 = C_9 = C_3 > C_7 = C_5 = C_4$) samples. The aromatic compound, benzoic acid, was detected in the adult and baby positive control samples (Shepherd & Dawson, unpublished data).

Long chain C_{16} fatty acids were not found in the samples, however, seven shorter chain free fatty acids in the range C_2 - C_9, acetic (C_2), propanoic (C_3), butanoic (C_4), hexanoic (C_6), heptanoic (C_7), octanoic (C_8) and nonanoic (C_9) acids were detected in the samples. In addition the aromatic compound benzoic acid was also present.

There is a sample location difference in the distribution of the C_2-C_9 acids which is related to acid chain length. The longer C_6-C_9 (hexanoic, heptanoic, octanoic and nonanoic) acids predominate at sample locations 7, 11, 14, 15 and 23, whereas the shorter C_2-C_4 (acetic, propanoic and butanoic)

acids predominate for samples 9, 14, 33, 45 and 49. Acetic and propanoic acids dominate the Northern boundary sample (53).
The aromatic benzoic acid has abundance maxima for samples 9, 14, 15, 33, 39 – 49 and for the Western (55) and Eastern (57) boundary samples.

Unsaturated aldehydes

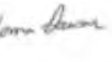
Unsaturated straight chain aldehydes, the 2-alkenals, have a double bond located between C2 and C3 of the alkyl chain. Six members of this series in the range $C_6 - C_{11}$ were found in the SPME positive control samples. These were in the general order of abundance $C_{10} > C_9 = C_8 > C_{11} > C_7 > C_6$, although the C_7 and C_9 homologues were not detected in the adult control samples. In addition, 2,4-nonadienal (C_9) with double bonds located between C2 and C3 and between C4 and C5, was also present in the adult and baby controls at abundance level intermediate between the C_{11} and C_6 2-alkenals (Shepherd & Dawson, unpublished data). The significance of the 2-alkenals with respect to mammalian decomposition is uncertain; however, their homologue distribution closely follows that of the equivalent saturated C_6 to C_{11} compounds, suggesting a common origin.

2-Alkenals in the range C_6 –C_{10} were detected in the samples, consisting of 2-hexenal (C_6), 2-heptenal (C_7), 2-octenal (C_8), 2-nonenal (C_9) and 2-decenal (C_{10}). In addition, 2,4-nonadienal (C_9) was also present.

The C_8-C_{10} unsaturated aldehydes 2-octenal, 2-nonenal and 2-decenal were most abundant, followed by the C_6 and C_7 compounds 2-hexenal and 2-heptenal and the C_9 2,4-nonadienal. This order of abundance is similar to that seen for the positive controls.
Abundance maxima were observed for samples 1-15, 23, 27, 33, 49, and for the Western boundary sample (55). This distribution profile is very similar to that seen for the saturated C_8-C_{10} *n*-aldehydes octanal, nonanal and decanal, providing further evidence for a common origin for both classes of compound.

Alkanes

Straight chain (*n*-) alkanes in the range C_5-C_{11} are associated with mammalian decomposition and the longer homologues are particularly associated with human decomposition, for which the presence of undecane (C_{11}) is considered to be a marker (Vaas et al., 2004, 2008; Vaas, 2012). Alkanes in the range C_7, C_9-C_{19} were found in the SPME positive control adult and baby samples with different abundance distributions for adult ($C_{12} > C_{10} = C_{13} = C_{14} > C_{16} = C_{15} > C_{17} > C_{11} = C_{18} = C_{19} > C_7 = C_9$) and baby ($C_{15} > C_{16} = C_{17} = C_{12} = C_{13} = C_{14} > C_{18} = C_{19} > C_{10} > C_{11} > C_7 = C_9$).
The C_{10}-C_{18} alkane homologues decane (C_{10}), Undecane (C_{11}), dodecane (C_{10}), tridecane (C_{13}), tetradecane (C_{14}), pentadecane (C_{15}), hexadecane (C_{16}) heptadecane (C_{17}) and octadecane (C_{18}) were found in the samples.

Signature...  ....Page 39 of 103

For most alkane homologues there is a broad abundance maxima profile over samples 1 – 15 and also at samples 23, 27, 31, 33 and 49, and at the Northern (53) and to a lesser extent the Western (55) boundary samples.

Maximum alkane abundances were seen for the longest C_{15}-C_{18} homologues, pentadecane, hexadecane, heptadecane and octadecane at the most easterly cell (sample 1), similar to the distribution seen for the positive control baby sample, and for tetradecane, hexadecane and octadecane at the Northern (53) boundary sample.

Undecane (C11) was generally of low abundance in all samples, but the abundance maxima for this compound were for samples 1-14, 23, 27, 31, 49, and for the boundary samples 53 and 55.

Data analysis

Analyte lists and analyte characterization

The first stage of data analysis was to create a master list of analytes of interest. This was based in part on published data describing volatiles associated with mammalian and human decomposition processes (Vaas et al., 2004, 2008; Vaas, 2012). In addition, further similar compounds were added following qualitative inspection of the data.

A composite sample analysis sequence was created using the Xcalibur™ software which allowed sequential qualitative inspection of all raw data files for all samples. Using this approach, combined selected ion chromatograms (SIC) for ion groups characteristic of specific target compounds were extracted and the SIC traces examined to assess for the presence of the target compounds in the sample. Ion groups for compound identification were selected by examination of reference MS data for the analytes in question which included published data, entries in commercial MS libraries and our own extensive databases. Selection criteria were that the ions should be of high relative abundance and where possible unique to the analyte, and should take into account possible contributions from overlapping and co-eluting analytes. In some instances it was necessary to modify the ion groups initially selected to provide optimal chromatographic resolution.

The master analyte list is shown in Table 2 and incorporates the following data:

(1) Name of analyte, and possible alternative identification(s);

(2) Retention time (R_t) (in minutes) and relative retention index (RRI);

(3) Molecular formula; molecular weight and the masses of the selected ions used for indentification and subsequent quantitation.

Relative retention index (RRI) describes the elution characteristics of analytes in a manner that is independent of the absolute retention times. It uses homologues of a specific class of compound, in this case straight chain saturated hydrocarbons (*n*-alkanes), as retention markers. Each alkane is assigned a RRI value of 100n where n is the number of carbon atoms in the alkane (e.g. octane, C_8, RRI = 800). Ideally a range of such alkanes differing in chain length by one carbon increments should be present in the analytical samples, or a mixture of such alkanes can be prepared, sampled and analysed separately under identical conditions. Each analyte is then assigned a calculated RRI value based on linear interpolation of the retention time differences between it and the two nearest adjacent alkane RRI markers of longer and shorter R_t. RRI values are therefore of greater utility when comparing retention data with that in pre-existing lists of metabolites previously analysed under similar conditions.

Automated data processing

An automated data processing method was created in Xcalibur™ using the data from the master metabolite list. This was used with the composite sample analysis sequence to extract then integrate the combined SIC trace of the diagnostic ions for each analyte within an analyte-specific defined time window, centered on the SIC peak apex. The output from the initial data processing was reviewed, checked for misidentification of peaks, and corrected where necessary. The results were then output to an excel workbook, with individual spreadsheets for each analyte in which the SIC peak areas were listed for each sample. This data was copied into a single spreadsheet listing analyte abundances against sample number. By comparison with the sample blanks many components present in each sample were shown to be sampling artifacts related to the SPME fiber chemistry and these were excluded from Tables 2 and 3. Compounds were identified by comparison of their mass spectra with entries in MS spectral libraries (NIST, Wiley and Pal600K), by comparison of mass spectral data and retention behavior with authentic standards and by extrapolation from data for known compounds. Where exact identities could not be given (e.g positional isomers with different substitution patterns) the general identity by compound family or class is given.

Table 1 Sampling Schedule

Sample Name	Context Number	Sample Weight (g)	Analysis Date	Analysis Time	Fibre No.	File Name
Lab control	Blank		11-Apr-17	09:47 AM	2	110417_IRS_SPME_PD_F2_blank_001
001	C.51	1.401	04-Apr-17	11.32 AM	2	040417_IRS_SPME_PD_F2_001_001_170404115644
003	C.53	2.019	04-Apr-17	12:49 PM	2	040417_IRS_SPME_PD_F2_003_001
005	C.55	2.447	04-Apr-17	14:02 PM	2	040417_IRS_SPME_PD_F2_005_001
007	C.57	1.667	04-Apr-17	15:15 PM	2	040417_IRS_SPME_PD_F2_007_001
009	C.59	3.220	04-Apr-17	16:28 AM	2	040417_IRS_SPME_PD_F2_009_001
011	C.61	1.855	04-Apr-17	17:40 PM	2	040417_IRS_SPME_PD_F2_011_001
013	C.63	1.734	05-Apr-17	10:01AM	3	050417_IRS_SPME_PD_F3_013_001
014	C.63	1.872	05-Apr-17	12:00 AM	3	050417_IRS_SPME_PD_F3_014_001
015	C.63	2.642	05-Apr-17	13:15 PM	3	050417_IRS_SPME_PD_F3_014_001_170405133831
017	C.65	3.090	05-Apr-17	14:27 PM	3	050417_IRS_SPME_PD_F3_014_001_170405145042
018	C.65	2.712	05-Apr-17	15:35 PM	3	050417_IRS_SPME_PD_F3_018_001
019	C.65	2.251	05-Apr-17	16:51 PM	3	050417_IRS_SPME_PD_F3_019_001
021	C.10	2.134	05-Apr-17	18:04 PM	3	050417_IRS_SPME_PD_F3_021_001
023	C.12	2.139	06-Apr-17	09:09 AM	3	060417_IRS_SPME_PD_F3_023_001
025	C.11	2.595	06-Apr-17	10:20 AM	3	060417_IRS_SPME_PD_F3_025_001
027	C.85	2.070	06-Apr-17	11:34 AM	3	060417_IRS_SPME_PD_F3_027_001
029	C.87	2.146	06-Apr-17	12:45 PM	3	060417_IRS_SPME_PD_F3_029_001
030	C.87	3.532	06-Apr-17	13:59 PM	3	060417_IRS_SPME_PD_F3_030_001
031	C.87	4.205	06-Apr-17	15:10 PM	3	060417_IRS_SPME_PD_F3_031_001
033	C.89	0.971	06-Apr-17	16:21 PM	3	060417_IRS_SPME_PD_F3_033_001
035	C.91	2.607	06-Apr-17	17:32 PM	3	060417_IRS_SPME_PD_F3_035_001
037	C.93	2.091	07-Apr-17	09:16 AM	3	070417_IRS_SPME_PD_F3_037_001
039	C.95	2.460	07-Apr-17	10:30 AM	3	070417_IRS_SPME_PD_F3_039_001
043	C.97	2.673	07-Apr-17	11:40 AM	3	070417_IRS_SPME_PD_F3_043_001
045	C.99	1.223	07-Apr-17	12:51 PM	3	070417_IRS_SPME_PD_F3_045_001
047	C.101	2.986	07-Apr-17	14:05 PM	3	070417_IRS_SPME_PD_F3_047_001
049	C.105	1.735	07-Apr-17	16:26 PM	2	070417_IRS_SPME_PD_F3_049b_001
051	C.2	3.523	07-Apr-17	17:39 PM	2	070417_IRS_SPME_PD_F2_051_001
053	N Boundary	2.608	07-Apr-17	18:50 PM	2	070417_IRS_SPME_PD_F2_053_001
055	W Boundary	2.277	10-Apr-17	12:04 PM	2	100417_IRS_SPME_PD_F2_055_001

Signature... ....Page 43 of 103

057	E Boundary	2.949	10-Apr-17	14:28 PM	2	100417_IRS_SPME_PD_F2_057_001
059	S Boundary	3.186	10-Apr-17	15:46 PM	2	100417_IRS_SPME_PD_F2_059_001

Signature... ....

Table 2. Compounds detected in soil samples

Best match(es)	Diagnostic ions	Formula	Mwt	Rt	RRI
Ethanol	45.1, 46.1	C_2H_6O	46	1.59	590
Dimethylsulfide	47.1, 62.1	C_2H_6S	62	1.60	591
Acetone	43.1, 58.1	C_3H_6O	58	1.68	601
Dichloromethane	49.1, 84.1, 86.1, 88.1	CH_2Cl_2	84	1.75	610
2,3-dihydrofuran[a]	39.1, 41.1, 69.1, 70.1	C_4H_6O	70	1.90	628
2-Methylpropanal	43.1, 72.1	C_4H_8O	72	1.94	633
2- or 3-Methylfuran	53.1, 81.1, 82.1	C_5H_6O	82	2.02	643
3- or 2-Methylfuran	53.1, 81.1, 82.1	C_5H_6O	82	2.13	657
Butanal	57.1, 72.1	C_4H_8O	72	2.24	670
2,3-Butanedione	43.1, 86.1	$C_4H_6O_2$	86	2.36	685
Tetrahydrofuran	42.1, 71.1, 72.1	C_4H_8O	72	2.38	686
Chloroform	83.1, 85.1, 87.1	$CHCl_3$	118	2.43	694
Benzene	51.1, 52.1, 78.1	C_6H_6	78	2.63	719
3-Methylbutanal	41.1, 43.1, 44.1, 57.1, 58.1, 71.1, 86.1	$C_5H_{10}O$	86	2.90	731
2-Methylbutanal	41.1, 43.1, 44.1, 57.1, 58.1, 71.1, 86.1	$C_5H_{10}O$	86	2.98	737
2-Ethylfuran	53.1, 81.1, 96.1	C_6H_8O	96	2.99	738
2-Pentanone[b]	43.1, 57.1, 71.1, 86.1	$C_5H_{10}O$	86	3.05	742
Pentanal	55.1, 57.1, 58.1	$C_5H_{10}O$	86	3.51	777
Acetic acid	43.1, 45.1, 60.1	$C_2H_4O_2$	60	3.74	794
Dimethyl disulfide	79.1, 94.1	$C_2H_6S_2$	94	3.97	809
Toluene	63.1, 65.1, 91.1, 92.1	C_7H_8	92	4.09	816
Pyridine	52.1, 79.1	C_5H_5N	79	4.40	834
2-Hexanone	43.1, 58.1, 71.1, 85.1, 100.1	$C_6H_{12}O$	100	5.17	880
Hexanal[c]	43.1, 44.1, 56.1, 57.1, 72.1, 82.1	$C_6H_{12}O$	100	5.21	883
Propanoic acid	45.1, 56.1, 57.1, 73.1, 74.1	$C_3H_6O_2$	74	5.25	885
Ethylbenzene[d]	65.1, 77.1, 91.1, 106.1	C_8H_{10}	106	5.70	912
Dimethylbenzene (1)[e]	65.1, 77.1, 91.1, 106.1	C_8H_{10}	106	5.83	919
Dimethylbenzene (2)[e]	65.1, 77.1, 91.1, 106.1	C_8H_{10}	106	6.33	948
Styrene	54.1, 78.1, 103.1, 104.1	C_8H_8	104	6.48	957
2-Hexenal	41.1, 55.1, 69.1, 83.1, 98.1	$C_6H_{10}O$	98	6.57	963
Butanoic acid	45.1, 60.1, 73.1, 88.1	$C_4H_8O_2$	88	6.70	970

Signature... ....

Table 2 (continued). Compounds detected in soil samples

Best match(es)	Diagnostic ions	Formula	Mwt	Rt	RRI
Furfural	39.1,67.1, 95.1, 96.1	$C_5H_4O_2$	96	6.72	971
1-hexanol'	41.1, 43.12, 56.1, 69.1, 84.1	$C_6H_{14}O_2$	102	6.85	979
2-Heptanone (MPK)	43.1, 58.1, 71.1, 85.1, 99.1, 114.1	$C_7H_{14}O$	114	6.92	983
Heptanal	43.1, 44.1, 57.1, 70.1, 71.1, 86.1, 96.1	$C_7H_{14}O$	114	6.98	987
Decane	43.1, 57.1, 71.1, 85.1, 99.1, 113.1, 142.2	$C_{10}H_{22}$	142	7.21	1000
Methylisopropylbenzene (1)	91.1, 119.1, 134.1	$C_{10}H_{14}$	134	7.33	1007
Methylethylbenzene[a]	91.1, 105.1, 120.1	C_9H_{12}	120	7.43	1013
2-Pentylfuran	53.1, 81.1,120.1, 138.1	$C_9H_{14}O$	138	7.78	1035
6-Methyl-2-heptanone	43.1, 58.1, 71.1, 95..1, 110.1, 128.1	$C_8H_{16}O$	128	7.99	1048
Ethylmethylbenzene[a]	91.1, 105.1, 120.1	C_9H_{12}	120	8.03	1050
2-Heptenal	41.1, 55.1, 70.1, 83.1, 97.1, 112.1	$C_7H_{12}O$	112	8.35	1070
Methylisopropylbenzene (2)	91.1, 119.1, 134.1	$C_{10}H_{14}$	134	8.42	1074
3-Octanone	43.1, 57.1, 71.1, 72.1, 99.1, 128.1	$C_8H_{16}O$	128	8.43	1075
Heptanol	55.1, 56.1, 69.1, 70.1, 83.1	$C_7H_{16}O$	116	8.52	1080
1-Octen-3-ol	43.1, 57.1, 72.1, 85.1, 99.1, 110.1, 128.1	$C_8H_{16}O$	128	8.53	1081
Benzaldehyde	51.1, 77.1, 105.1, 106.1	C_7H_6O	106	8.59	1085
2-Octanone	43.1, 55.1, 58.1, 71.1, 85.1, 113.1, 128.1	$C_8H_{16}O$	128	8.60	1085
6-Methyl-5-hepten-2-one	41.1, 43.1, 55.1, 58.1, 69.1, 93.1, 108.1, 111.1,126.1	$C_8H_{14}O$	126	8.61	1086
Octanal	43.1, 44.1, 57.1, 69.1, 84.1, 100.1, 110.1	$C_8H_{16}O$	128	8.69	1091
Undecane	43.1, 57.1, 71.1, 85.1, 99.1, 113.1, 156.2	$C_{11}H_{24}$	156	8.84	1100
Dimethylstyrene (2)'	91.1, 115.1, 117.1, 132.1	$C_{10}H_{20}O$	132	9.68	1155
Hexanoic acid	41.1, 60.1, 73.1, 87.1, 98.1	$C_6H_{12}O_2$	116	9.78	1162
2-Octenal	5.1, 69.1, 70.1, 83.1, 97.1, 108.1, 111.1, 126.1	$C_8H_{14}O$	126	9.99	1175
1-Octanol	55.1, 56.1, 69.1, 70.1, 83.1, 84.1, 97.1, 112.1	$C_8H_{18}O$	130	10.06	1180
Phenylacetaldehyde	65.1, 91.1, 120.1	C_8H_8O	120	10.13	1184
2-Nonanone	43.1, 58.1, 71.1, 142.1	$C_9H_{18}O$	142	10.19	1188
Nonanal	43.1, 55.1, 57.1, 67.1, 70.1, 82.1, 95.1, 98.1, 114.1	$C_9H_{18}O$	142	10.28	1194
Dodecane	43.1, 57.1, 71.1, 85.1, 99.1, 113.1, 156.2	$C_{12}H_{26}$	170	10.37	1200
Acetophenone	77.1, 105.1, 120.1	C_8H_8O	120	10.43	1204
Phenol	65.1, 66.1, 94.1	C_6H_6O	94	10.68	1222
Heptanoic acid	60.1, 73.1, 87.1, 101.1, 113.1	$C_7H_{14}O_2$	130	11.16	1255

Table 2 (continued). Compounds detected in soil samples

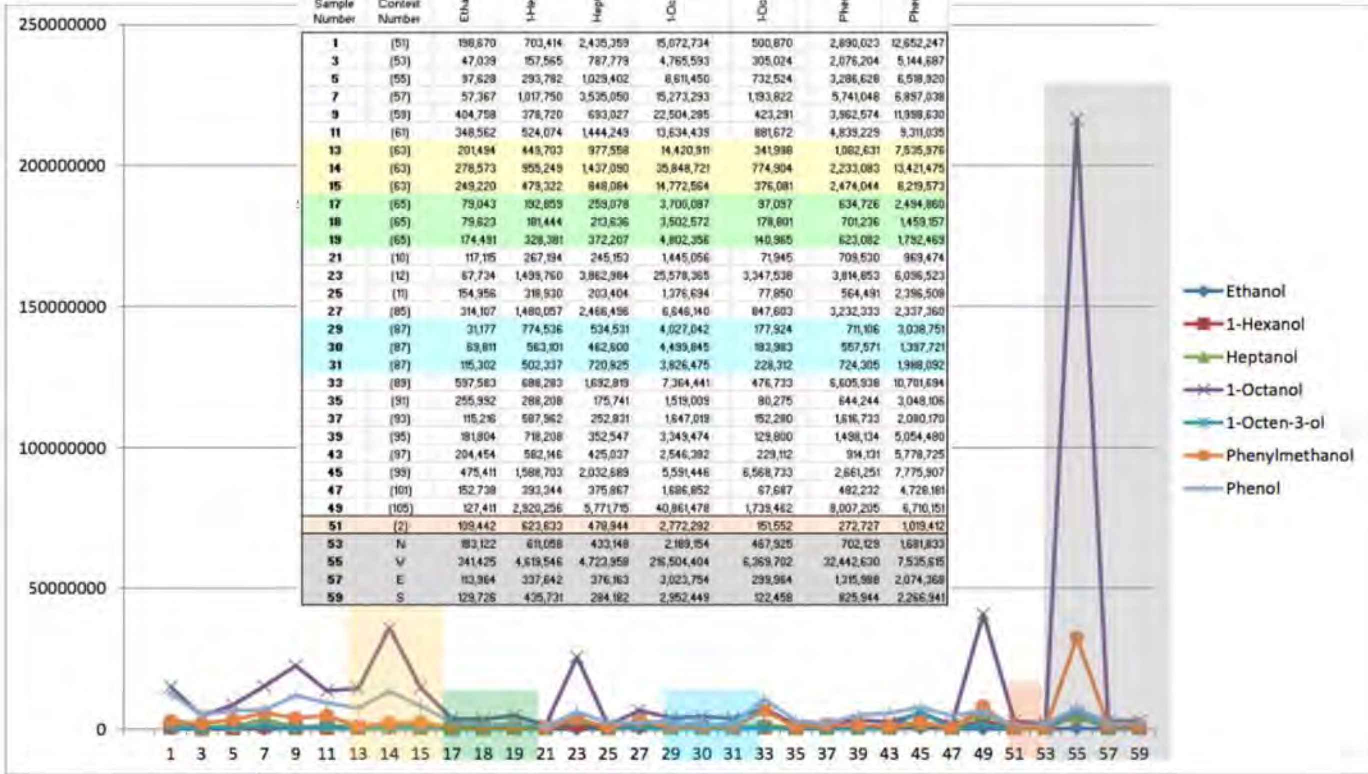
Best match(es)	Diagnostic ions	Formula	Mwt	Rt	RRI
2-Nonenal	41.1, 55.1, 70.1, 83.1, 97.1, 111.1, 127.1	$C_9H_{16}O$	140	11.52	1280
Phenylmethanol	91.1, 92.1, 122.1	$C_8H_{10}O$	122	11.56	1283
2-Decanone	43.1, 58.1, 96.1, 98.1, 113.1, 141.1, 156.2	$C_{10}H_{20}O$	156	11.68	1292
Decanal	43.1, 55.1, 57.1, 67.1, 70.1, 82.1, 95.1, 112.1, 128.1	$C_{10}H_{20}O$	156	11.77	1298
Tridecane	57.1, 71.1, 85.1, 99.1, 113.1, 184.1	$C_{13}H_{28}$	184	11.80	1300
Octanoic acid	60.1, 73.1, 85.1, 101.1, 115.1, 129.1, 144.1	$C_8H_{16}O_2$	144	12.51	1352
2, 4-Nonadienal	67.10, 81.10, 95.10, 138.10	$C_9H_{14}O$	138	12.55	1355
2-Decenal	41.1, 43.1, 55.1, 70.1, 83.1, 98.1, 110.1, 121.1, 136.1	$C_{10}H_{18}O$	154	12.96	1385
2-Undecanone	43.1, 58.1, 71.1, 85.1, 113.1, 155.1, 170.2	$C_{11}H_{22}O$	170	13.07	1394
Tetradecane	43.1, 57.1, 71.1, 85.1, 99.1, 113.1, 127.1, 141.1	$C_{14}H_{30}$	198	13.17	1400
Undecanal	43.1, 55.1, 57.1, 69.1, 70.1, 82.1, 96.1, 11.1, 126.1, 142.1, 152.1	$C_{11}H_{22}O$	170	13.19	1402
Benzoic acid	77.1, 105.1, 122.1	$C_7H_6O_2$	122	13.27	1408
Nonanoic acid	60.1, 73.1, 85.1, 98.1, 115.1, 129.1, 158.2	$C_9H_{18}O_2$	158	13.80	1449
2-Dodecanone	43.1, 58.1, 71.1, 85.1, 110.1, 169.1, 184.2	$C_{12}H_{24}O$	184	13.92	1459
Dodecanal (b)	43.1, 55.1, 57.1, 69.1, 70.1, 82.1, 96.1, 110.1, 126.1, 140.1, 156.1	$C_{12}H_{24}O$	184	14.03	1467
Pentadecane	57.1, 71.1, 85.1, 99.1, 113.1, 127.1, 141.1, 226.2	$C_{15}H_{32}$	212	14.44	1500
Hexadecane	57.1, 71.1, 85.1, 99.1, 113.1, 127.1, 141.1, 226.3	$C_{16}H_{34}$	226	15.64	1600
2-Tridecanone	43.10, 58.10, 71.10, 85.10, 96.1, 110.10, 140.10, 183.20, 198.2	$C_{13}H_{26}O$	198	15.65	1601
Heptadecane	57.1, 71.1, 85.1, 99.1, 113.1, 127.1, 141.1, 240.3	$C_{17}H_{36}$	240	16.79	1700
Pentadecanal	43.10, 55.10, 57.10, 69.10, 70.10, 82.10, 96.10, 110.10, 124.10, 137.10, 152.10	$C_{15}H_{30}O$	226	17.64	1779
Octadecane	57.1, 71.1, 85.1, 99.1, 113.1, 127.1, 141.1, 254.3	$C_{18}H_{38}$	254	17.87	1800

Alternative matches: [a]2- or 3-Butenal; [b]3-Me-2-butanone; [c]1-hexen-3-ol; [d]Dimethylbenzene; [e]Ethylbenzene; [f]4-Methyl-1-pentanol; [g]Trimethylbenzene or Propylbenzene; [h]Methyl propenylbenzene.

Signature... *[signature]* ....

Table 3. Aliphatic and aromatic alcohols and phenol (abundance per g of sample)

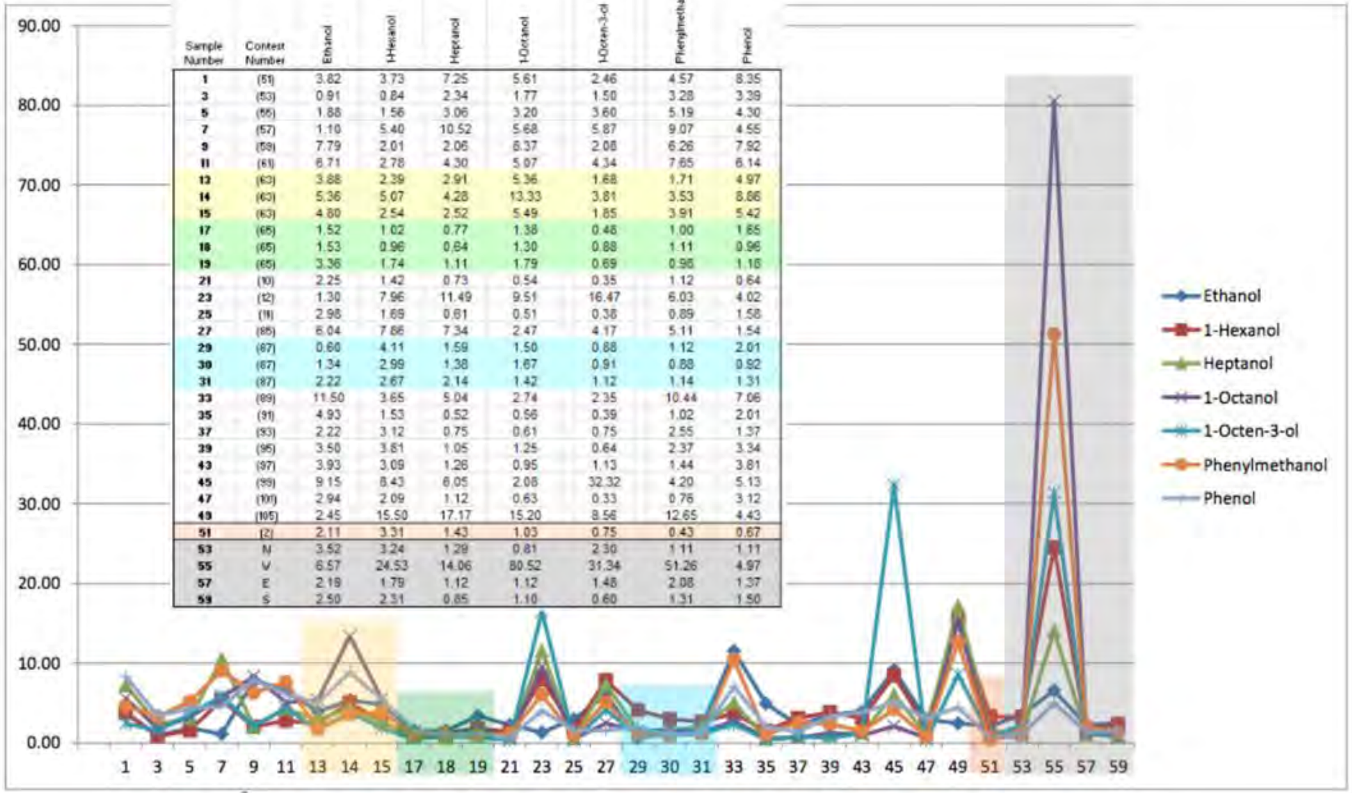
Sample Number	Context Number	Ethanol	1-Hexanol	Heptanol	1-Octanol	1-Octen-3-ol	Phenylmethanol	Phenol
1	(51)	198,670	703,414	2,435,359	15,072,734	500,870	2,890,023	12,652,247
3	(53)	47,039	157,565	787,779	4,765,593	305,024	2,076,204	5,144,687
5	(55)	97,628	293,782	1,029,402	8,611,450	732,524	3,286,628	6,518,920
7	(57)	57,367	1,017,750	3,535,050	15,273,293	1,193,822	5,741,048	6,897,038
9	(59)	404,758	378,720	693,027	22,504,285	423,291	3,962,574	11,998,630
11	(61)	348,562	524,074	1,444,249	13,634,439	881,672	4,839,229	9,311,035
13	(63)	201,494	449,703	977,558	14,420,911	341,998	1,082,631	7,535,976
14	(63)	278,573	955,249	1,437,090	35,848,721	774,904	2,233,083	13,421,475
15	(63)	249,220	479,322	848,084	14,772,564	376,081	2,474,044	8,219,573
17	(65)	79,043	192,859	259,078	3,700,087	97,097	634,726	2,494,860
18	(65)	79,623	181,444	213,636	3,502,572	178,801	701,236	1,459,157
19	(65)	174,491	328,381	372,207	4,802,356	140,965	623,082	1,792,469
21	(10)	117,115	267,194	245,153	1,445,056	71,945	709,530	969,474
23	(12)	67,724	1,499,760	3,862,984	25,578,365	3,347,538	3,814,853	6,096,523
25	(11)	154,956	318,930	203,404	1,376,694	77,850	564,491	2,396,509
27	(85)	314,107	1,480,057	2,466,496	6,646,140	847,603	3,232,333	2,337,360
29	(87)	31,177	774,536	534,531	4,027,042	177,924	711,106	3,038,751
30	(87)	69,811	563,101	462,600	4,499,845	183,983	557,571	1,397,721
31	(87)	115,302	502,337	720,925	3,826,475	228,312	724,305	1,988,092
33	(89)	597,583	686,283	1,692,819	7,364,441	476,733	6,605,938	10,701,694
35	(91)	255,992	288,208	175,741	1,519,009	80,275	644,244	3,048,106
37	(93)	115,216	587,962	252,831	1,647,019	152,280	1,616,733	2,080,170
39	(95)	181,804	718,208	352,547	3,349,474	129,800	1,498,134	5,054,480
43	(97)	204,454	582,146	425,037	2,546,392	229,112	914,131	5,779,725
45	(99)	475,411	1,588,703	2,032,689	5,591,446	6,568,733	2,661,251	7,775,907
47	(101)	152,738	393,244	375,867	1,686,852	67,687	482,232	4,728,181
49	(105)	127,411	2,920,256	5,771,715	40,861,478	1,739,462	8,007,205	6,710,151
51	(2)	109,442	623,633	478,944	2,772,292	151,552	272,727	1,019,412
53	N	183,122	611,058	433,148	2,189,154	467,925	702,129	1,681,833
55	V	341,425	4,619,546	4,723,959	216,504,404	6,369,702	32,442,630	7,535,615
57	E	113,964	337,642	376,163	3,023,754	299,964	1,315,988	2,074,368
59	S	129,726	435,731	284,182	2,952,449	122,458	825,944	2,266,941



Signature... ....Page 48 of 103

Table 3 (continued). Aliphatic and aromatic alcohols and phenol (abundance per sample as a percentage of the total abundance for samples 1 – 49)

Sample Number	Contest Number	Ethanol	1-Hexanol	Heptanol	1-Octanol	1-Octen-3-ol	Phenylmethanol	Phenol
1	(51)	3.82	3.73	7.25	5.61	2.46	4.57	8.35
3	(53)	0.91	0.84	2.34	1.77	1.50	3.28	3.39
5	(55)	1.88	1.56	3.06	3.20	3.60	5.19	4.30
7	(57)	1.10	5.40	10.52	5.68	5.87	9.07	4.55
9	(59)	7.79	2.01	2.06	6.37	2.08	6.26	7.92
11	(61)	6.71	2.78	4.30	5.07	4.34	7.65	6.14
13	(63)	3.88	2.39	2.91	5.36	1.68	1.71	4.97
14	(63)	5.36	5.07	4.28	13.33	3.81	3.53	8.86
15	(63)	4.80	2.54	2.52	5.49	1.85	3.91	5.42
17	(65)	1.52	1.02	0.77	1.38	0.48	1.00	1.65
18	(65)	1.53	0.96	0.64	1.30	0.88	1.11	0.96
19	(65)	3.36	1.74	1.11	1.79	0.69	0.98	1.18
21	(10)	2.25	1.42	0.73	0.54	0.35	1.12	0.64
23	(12)	1.30	7.96	11.49	9.51	16.47	6.03	4.02
25	(11)	2.98	1.69	0.61	0.51	0.38	0.89	1.58
27	(85)	6.04	7.66	7.34	2.47	4.17	5.11	1.54
29	(87)	0.60	4.11	1.59	1.50	0.88	1.12	2.01
30	(87)	1.34	2.99	1.38	1.67	0.91	0.88	0.92
31	(87)	2.22	2.67	2.14	1.42	1.12	1.14	1.31
33	(89)	11.50	3.65	5.04	2.74	2.35	10.44	7.06
35	(91)	4.93	1.53	0.52	0.56	0.39	1.02	2.01
37	(93)	2.22	3.12	0.75	0.61	0.75	2.55	1.37
39	(95)	3.50	3.81	1.05	1.25	0.64	2.37	3.34
43	(97)	3.93	3.09	1.26	0.95	1.13	1.44	3.81
45	(99)	9.15	8.43	6.05	2.08	32.32	4.20	5.13
47	(101)	2.94	2.09	1.12	0.63	0.33	0.76	3.12
49	(105)	2.45	15.50	17.17	15.20	8.56	12.65	4.43
51	(2)	2.11	3.31	1.43	1.03	0.75	0.43	0.67
53	N	3.52	3.24	1.29	0.81	2.30	1.11	1.11
55	V	6.57	24.53	14.06	80.52	31.34	51.26	4.97
57	E	2.18	1.79	1.12	1.12	1.48	2.08	1.37
59	S	2.50	2.31	0.85	1.10	0.60	1.31	1.50



Signature... ....Page 49 of 103

Table 3 (continued). Aliphatic and aromatic alcohols and phenol

- The aliphatic alcohols ethanol (C_2), 1-hexanol (C_6), 1-heptanol (C_7) and the aromatic compound phenol were found in the samples, along with the C_8 alcohols 1-octanol and 1-octen-3-ol, and the aromatic alcohol phenyl methanol.

- In terms of abundance per g of sample and proportional abundance, hotspots are found for phenol and phenylmethanol in samples 7 – 15, 23, 33, and 39-45. Collectively for ethanol, 1-hexanol and 1-heptanol, hotspots are found for samples 7, 9, 11, 23, 27, 33, 45 and 49. Hotspots for 1-octanol and 1-octen-3-ol were found for samples 7-15, 23, 45 and 49.

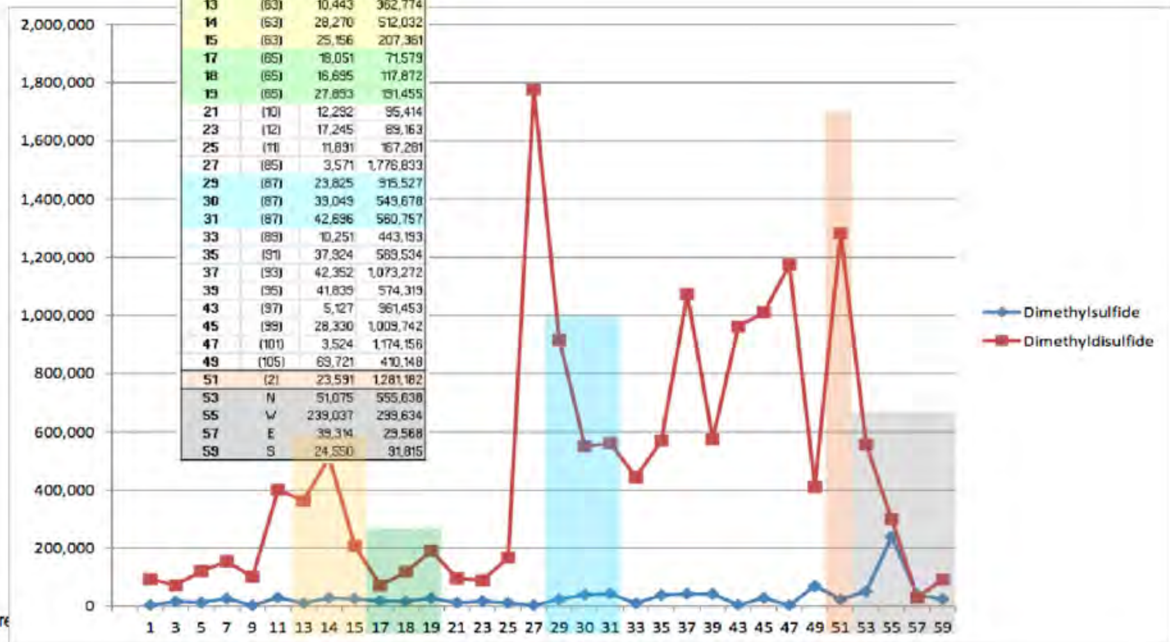
- High abundances of these compounds, particularly phenyl methanol and the C_8 alcohols were also found for the West boundary control sample (55).

- Abundances of these compounds were low in one of the cells with no visible human remains (samples 17 – 19), but showed a peak for some components in the other (samples 13 – 15).

- Ethanol, 1-pentanol, 1-hexanol, 1-heptanol and phenol are known non-specific markers of bone decomposition in mammals

Table 3 (continued). Sulfur Compounds (abundance per g of sample)

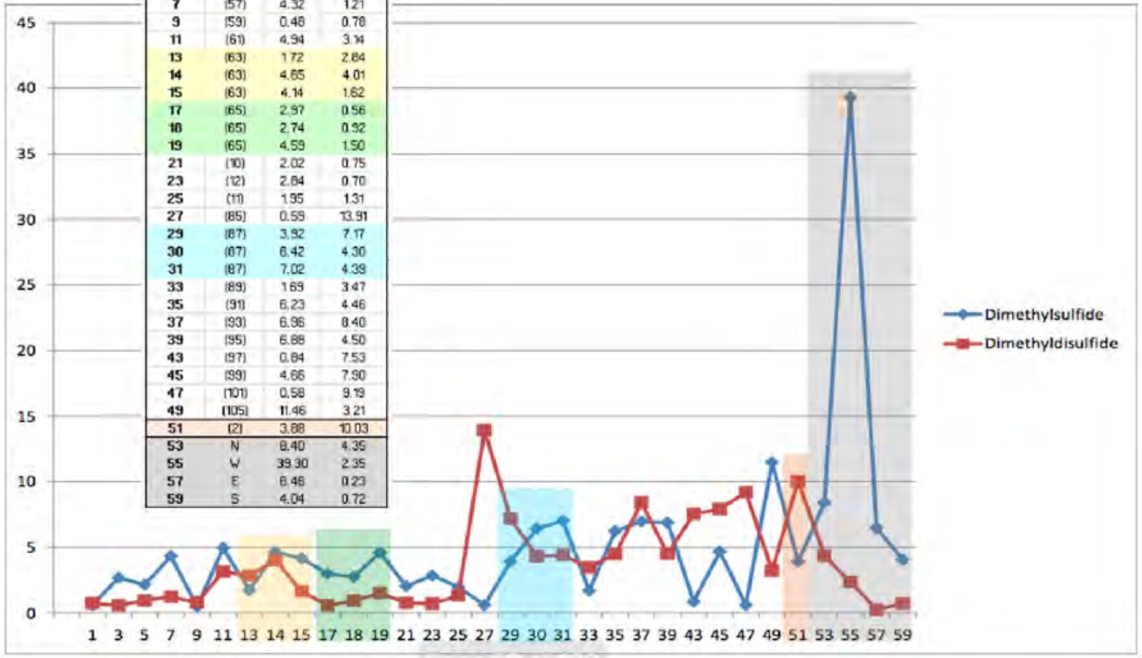
Sample Number	Context Number	Dimethylsulfide	Dimethyldisulfide
1	(51)	3,636	93,267
3	(53)	16,246	72,412
5	(55)	13,040	120,593
7	(57)	26,275	154,340
9	(59)	2,907	100,140
11	(61)	30,029	400,844
13	(63)	10,443	362,774
14	(63)	28,270	512,032
15	(63)	25,156	207,361
17	(65)	18,051	71,579
18	(65)	16,695	117,872
19	(65)	27,853	191,455
21	(10)	12,292	95,414
23	(12)	17,245	89,163
25	(11)	11,891	167,281
27	(85)	3,571	1,776,833
29	(87)	23,825	915,527
30	(87)	39,049	549,678
31	(87)	42,696	560,757
33	(89)	10,251	443,193
35	(91)	37,924	569,534
37	(93)	42,352	1,073,272
39	(95)	41,839	574,319
43	(97)	5,127	961,453
45	(99)	28,330	1,009,742
47	(101)	3,524	1,174,156
49	(105)	69,721	410,148
51	(2)	23,591	1,281,182
53	N	51,075	555,638
55	W	239,037	299,634
57	E	39,314	29,568
59	S	24,550	91,815



Signatur

Table 3 (continued). Sulfur Compounds (abundance per sample a percentage of the total abundance for samples 1 – 49)

Sample Number	Context Number	Dimethylsulfide	Dimethyldisulfide
1	(51)	0.60	0.73
3	(53)	2.67	0.57
5	(55)	2.14	0.94
7	(57)	4.32	1.21
9	(59)	0.48	0.78
11	(61)	4.94	3.14
13	(63)	1.72	2.84
14	(63)	4.65	4.01
15	(63)	4.14	1.62
17	(65)	2.97	0.56
18	(65)	2.74	0.92
19	(65)	4.59	1.50
21	(10)	2.02	0.75
23	(12)	2.84	0.70
25	(11)	1.95	1.31
27	(85)	0.59	13.91
29	(87)	3.92	7.17
30	(87)	6.42	4.30
31	(87)	7.02	4.39
33	(89)	1.69	3.47
35	(91)	6.23	4.46
37	(93)	6.96	8.40
39	(95)	6.88	4.50
43	(97)	0.84	7.53
45	(99)	4.66	7.90
47	(101)	0.58	9.19
49	(105)	11.46	3.21
51	(2)	3.88	10.03
53	N	8.40	4.35
55	W	39.30	2.35
57	E	6.46	0.23
59	S	4.04	0.72



Signature... ....Page 52 of 103

Table 3 (continued). Sulfur Compounds

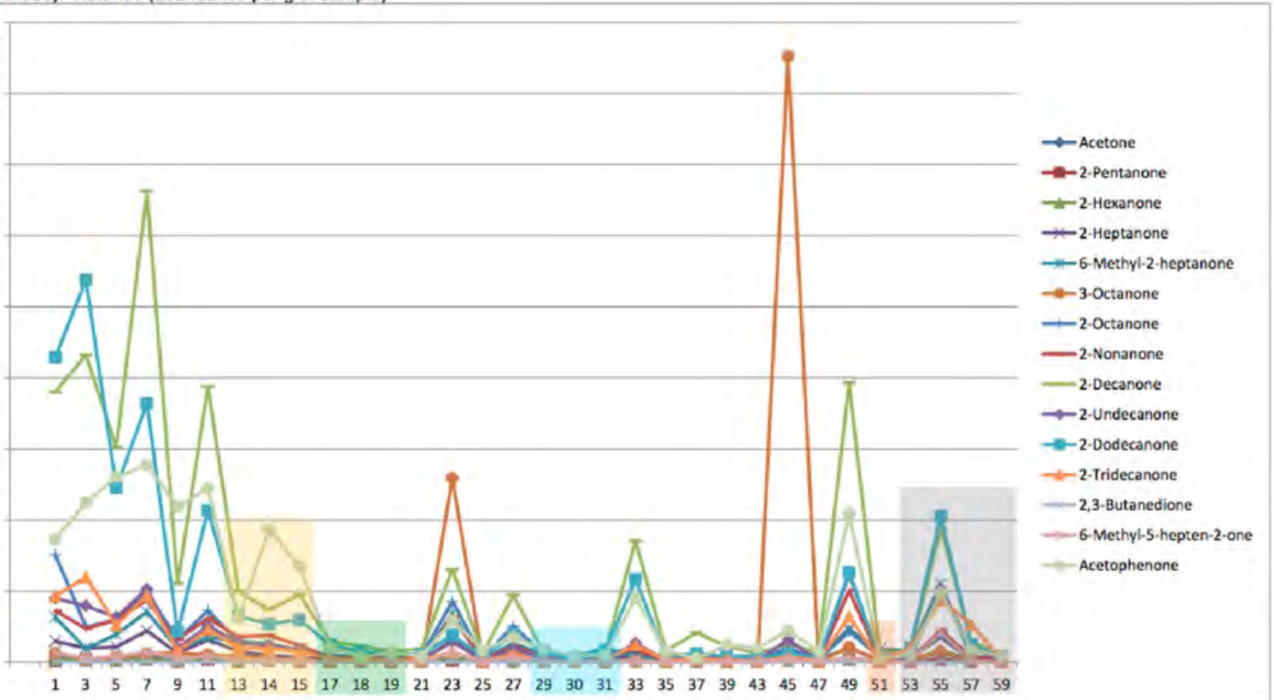
- Dimethylsulfide (DMS) and dimethyldisulfide (DMDS) were the only sulfur compounds detected in the samples. These compounds are non-specific markers of mammalian decomposition.
- Proportional abundance and abundance per g for DMS is fairly uniform across the samples with perhaps an indication of an increase for cells located towards the west (higher sample number). The abundance for this compound is significantly greater for the West boundary sample (55).
- The abundance profiles for DMDS show maxima for samples 11-14, the west tending samples 27-49, the Baulk sample (51) and to a lesser extent North boundary control (53). The abundances of DMDS in the other boundary samples, including the West boundary sample (55) are relatively low in comparison.
- Abundances of DMDS compounds were low in one of the cells with no visible human remains (samples 17 – 19), but showed a peak in the other (samples 13 – 15).

Table 3 (continued). Ketones (abundance per g of sample)

Sample Number	Context Number	Acetone	2-Pentanone	2-Hexanone	2-Heptanone	6-Methyl-2-heptanone	3-Octanone	2-Octanone	2-Nonanone	2-Decanone	2-Undecanone	2-Dodecanone	2-Tridecanone	2,3-Butanedione	6-Methyl-5-hepten-2-one	Acetophenone
1	(51)	1,870,360	372,203	855,951	5,947,551	12,645,800	2,632,180	30,241,629	14,438,808	75,979,660	17,943,975	85,726,580	18,568,544	34,320	2,592,651	34,552,743
3	(53)	686,744	601,281	655,937	3,918,304	3,787,312	817,146	9,903,138	9,477,006	86,353,429	15,859,018	107,524,623	23,893,510	78,976	1,096,780	44,951,164
5	(55)	1,064,193	498,050	621,718	4,273,981	7,852,481	1,264,130	11,815,082	11,940,728	60,438,793	12,648,662	49,038,373	10,483,608	35,973	1,610,550	52,076,126
7	(57)	2,099,956	849,544	1,086,201	8,827,971	14,167,259	2,353,913	19,627,215	17,492,118	132,501,086	20,574,067	72,861,215	18,803,213	75,858	2,809,026	55,440,289
9	(59)	240,254	225,511	470,372	2,549,047	3,786,668	2,575,505	6,356,083	6,368,953	22,101,142	3,942,459	8,709,159	3,143,546	30,060	1,016,837	43,730,224
11	(61)	1,318,244	798,588	1,160,981	6,392,556	7,091,725	2,091,827	14,507,531	12,391,933	77,508,475	10,197,226	42,658,697	9,145,642	67,903	1,857,245	48,906,075
13	(63)	1,935,191	200,527	399,906	3,114,641	5,863,772	1,703,481	5,687,533	7,147,211	19,921,642	5,442,133	12,938,979	4,193,558	46,812	804,023	12,393,612
14	(63)	1,521,573	460,075	608,535	1,862,594	5,220,519	913,730	4,986,352	7,581,940	14,821,462	4,569,503	10,741,560	3,765,962	43,416	645,910	37,240,387
15	(63)	1,139,590	234,025	465,012	1,399,973	3,166,242	592,010	3,011,329	4,741,812	18,942,404	3,741,927	11,943,093	2,949,121	46,060	425,186	27,009,585
17	(65)	806,372	169,633	172,562	619,942	1,742,795	214,998	1,498,191	1,219,368	5,853,652	883,026	4,869,787	1,023,938	25,231	193,090	4,253,434
18	(65)	1,475,090	314,982	244,699	1,403,600	2,001,179	353,254	1,780,740	1,138,000	4,636,880	676,864	3,066,600	737,093	42,610	235,650	1,462,488
19	(65)	1,624,731	218,762	263,374	887,584	1,812,688	199,873	1,611,195	1,249,005	3,015,395	629,235	2,270,059	533,717	43,650	243,347	2,653,818
21	(10)	1,269,391	252,442	171,042	727,143	1,069,236	219,415	1,834,340	918,386	3,771,837	543,680	2,130,066	724,108	40,233	179,950	1,653,966
23	(12)	1,589,156	491,720	1,215,148	6,249,031	13,694,058	51,722,675	17,112,663	12,722,578	26,023,768	5,635,632	7,615,238	2,772,029	65,939	2,717,333	11,708,801
25	(11)	657,209	156,318	235,439	885,144	1,036,482	219,506	1,155,248	662,025	2,393,396	387,220	1,628,284	319,996	29,003	125,041	3,474,688
27	(85)	131,717	321,465	480,825	3,568,589	5,303,446	2,525,323	10,248,745	4,487,053	18,908,058	3,690,572	7,696,778	2,151,905	12,039	1,501,722	7,064,693
29	(87)	1,032,638	226,268	297,819	1,517,496	2,192,428	469,551	2,059,511	1,500,167	2,570,017	817,224	3,110,223	444,264	57,410	213,890	3,700,372
30	(87)	554,636	103,448	211,753	995,717	1,601,812	148,742	1,538,807	1,633,107	1,888,427	362,225	677,092	132,878	32,377	208,209	1,620,178
31	(87)	272,156	108,280	225,440	841,601	3,862,875	348,527	1,981,958	1,759,359	2,691,332	405,725	3,124,742	478,844	14,436	298,904	2,006,469
33	(89)	1,976,955	996,032	242,668	2,407,555	1,571,614	243,410	4,305,965	3,658,487	34,094,464	5,425,416	23,306,975	4,943,593	101,308	561,710	18,118,044
35	(91)	901,610	219,081	95,167	885,520	604,781	106,872	595,338	530,108	3,274,147	527,816	1,590,038	475,035	71,210	90,882	2,979,790
37	(93)	948,221	175,652	252,462	1,263,228	1,017,481	410,889	1,124,375	1,002,718	8,311,753	1,549,205	2,402,526	887,486	60,534	195,561	1,091,195
39	(95)	1,007,151	150,251	245,225	1,071,317	1,629,823	114,397	1,306,267	1,440,380	4,428,593	754,786	1,629,520	630,913	25,739	164,005	4,756,023
43	(97)	835,368	220,454	166,911	1,318,843	1,715,897	221,099	1,243,455	879,689	2,427,595	316,358	924,892	300,998	21,642	265,598	4,051,178
45	(99)	3,954,063	3,615,161	404,896	2,905,124	2,364,567	170,415,316	3,354,755	2,203,498	5,278,920	6,342,879	2,500,887	1,349,191	172,533	694,779	8,865,141
47	(101)	660,138	90,312	73,750	707,457	695,581	91,779	702,907	391,590	2,512,552	401,891	1,125,925	369,060	13,242	109,046	3,040,413
49	(105)	3,969,537	743,732	941,505	9,584,978	9,010,425	4,240,477	8,612,480	20,134,204	78,572,557	24,747,645	25,276,427	12,880,381	187,469	1,353,983	41,627,252
51	(2)	520,522	183,467	279,575	1,346,315	3,535,801	352,746	1,573,439	826,431	2,743,088	633,262	918,032	365,219	52,870	202,454	981,207
53	N	1,063,998	270,862	525,462	1,068,203	3,403,871	504,452	1,160,025	617,839	3,142,298	1,188,041	4,061,976	4,087,375	44,831	230,600	2,139,919
55	V	2,487,958	807,758	3,341,613	7,075,530	21,970,113	2,971,933	7,980,899	9,137,500	37,600,106	20,687,217	41,037,989	17,523,022	48,984	8,449,828	19,513,766
57	E	482,756	174,534	604,310	556,323	1,245,718	256,472	1,067,149	1,389,038	5,749,472	3,726,375	4,917,454	10,640,520	19,405	305,911	3,376,633
59	S	594,626	194,897	365,127	701,215	1,672,530	94,110	725,037	817,636	2,366,627	865,824	1,436,579	597,950	24,420	135,495	1,817,673

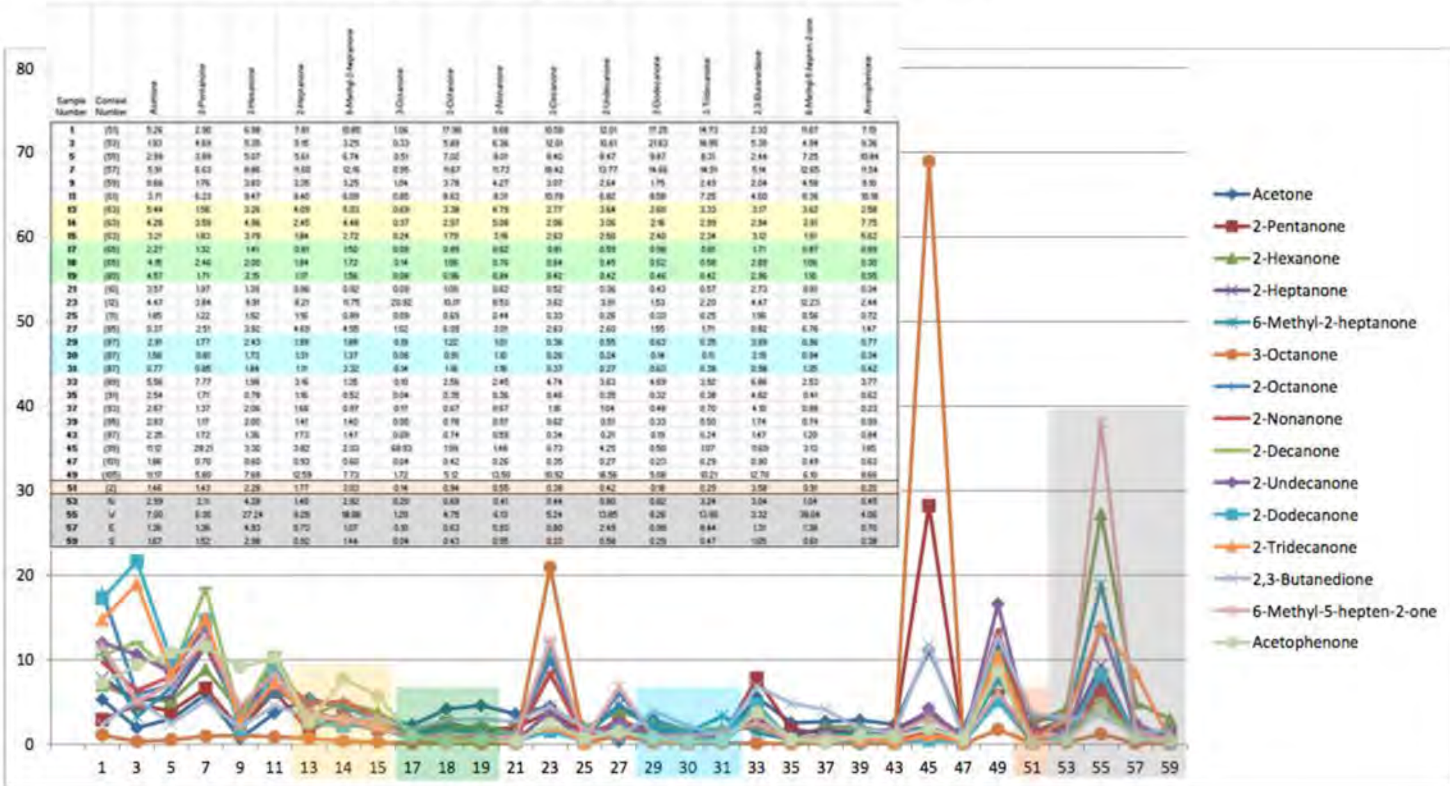
Signature... ....Page 54 of 103

Table 3 (continued). Ketones (abundance per g of sample)



Signature... ....Page 55 of 103

Table 3 (continued). Ketones (abundance per sample as a percentage of the total abundance for samples 1 – 49)



Signature... ....Page 56 of 103

Table 3 (continued). Ketones

- A range of aliphatic ketones in the range C_3-C_{13} with the keto group at the C-2 position in the alkyl chain were detected in the samples. These include 2-propanone (acetone, C_3), 2-pentanone (C_5), 2-hexanone (C_6), 2-heptanone (C_7), 2-octanone (C_8), 2-nonanone (C_9), 2-decanone (C_{10}), 2-undecanone (C_{11}), 2-dodecanone (C_{12}) and 2-tridecanone (C_{13}). In addition the branched saturated and unsaturated C_8 homologues of this series, 6-methyl-2-heptanone and 6-methyl-5-hepten-2-one, were also found along with the C_8 compound 3-octanone, which has the keto group at C-3. A C_4 diketo compound, 2,3-butanedione and an aromatic ketone acetophenone were also present.

- Abundance hotspots for the C-2 ketones were found for samples 1-11, 23, 27, 33, 45 and 49, particularly for 2-decanone (C_{10}), 2-undecanone (C_{11}), and to a lesser extent for 2-pentanone (C_5), 2-octanone (C_8) and 2-nonanone (C_9). Higher levels of the C-3 ketone 3-octanone (C_8) were associated with samples 23 and 45.

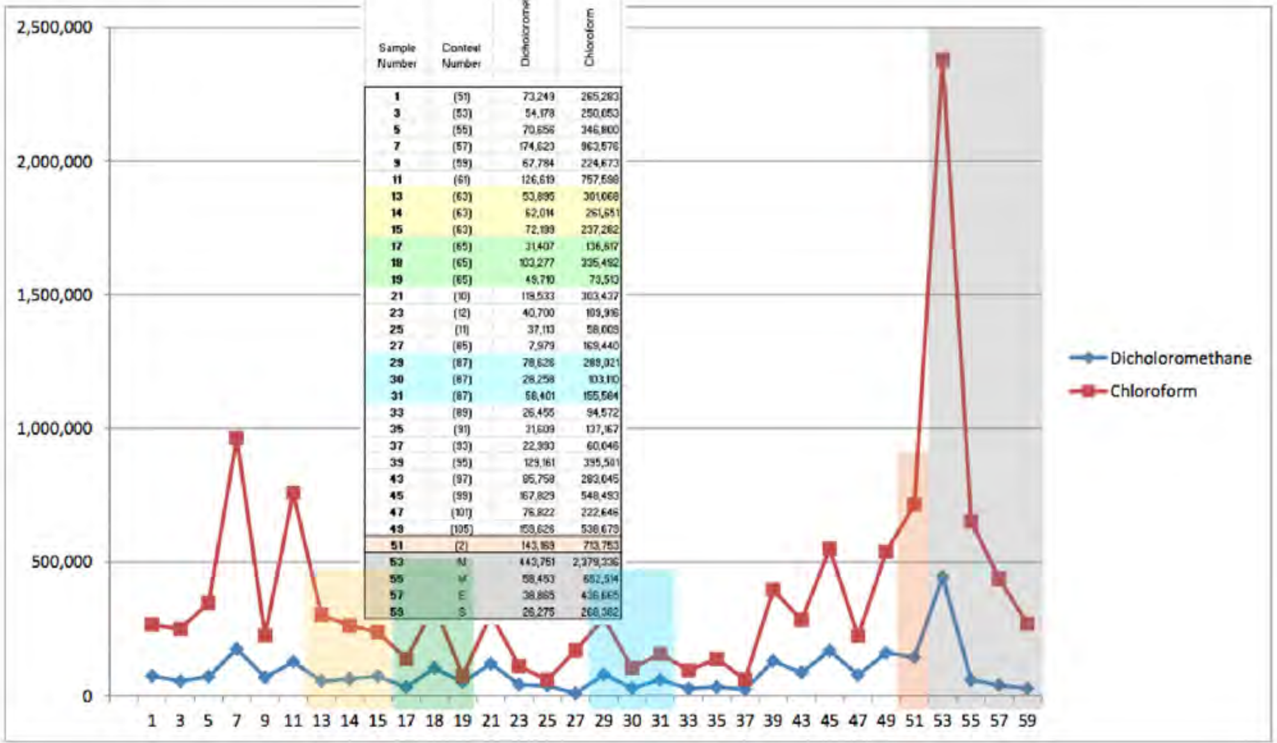
- The western control also showed appreciable abundances of some of these compounds, particularly 2-hexanone (C_6) and the branched C_8 compounds 6-methyl-2-heptanone and 6-methyl-5-hepten-2-one.

- Ketones were generally of lower abundance in one of the samples from cells with no visible human remains (17-19), but were of higher abundance for some components in the other (samples 13 – 15).

- Acetone 2-nonanone and 2-decanone are associated with human and other mammalian decomposition, particularly of bone.

Table 3 (continued). Halocarbons (abundance per g of sample)

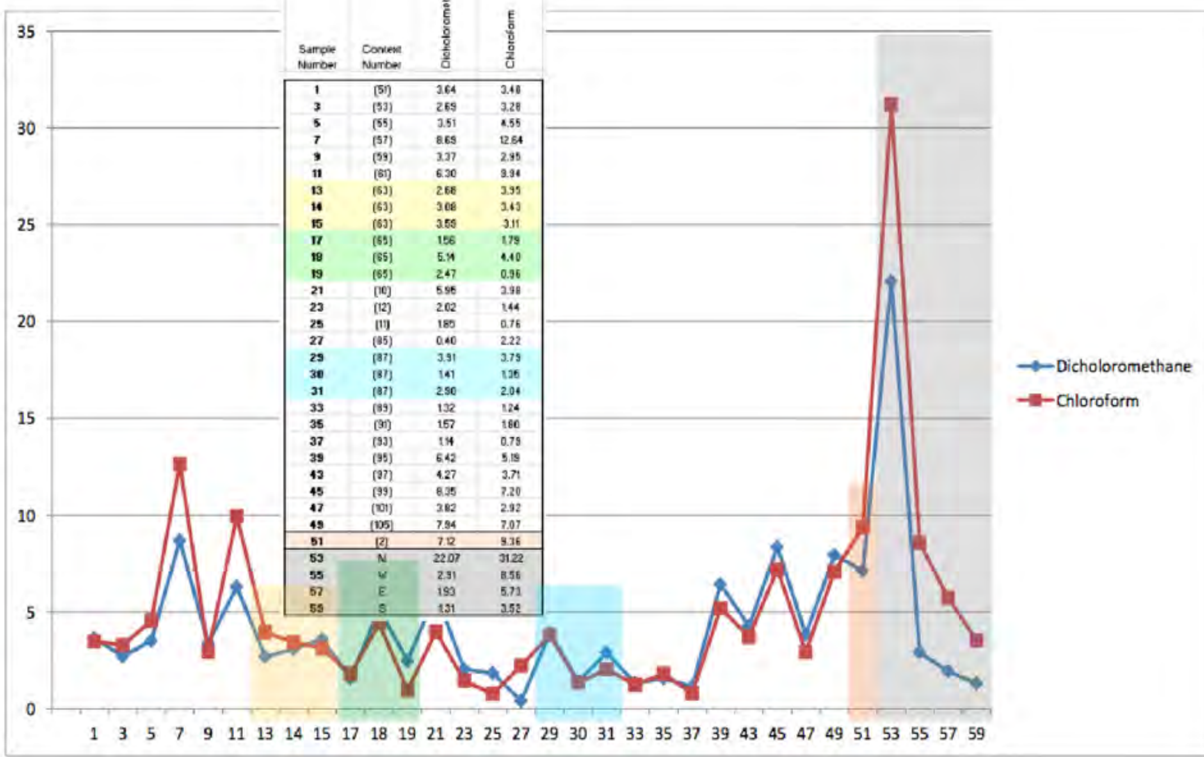
Sample Number	Context Number	Dicholoromethane	Chloroform
1	(51)	73,249	265,283
3	(53)	54,178	250,653
5	(55)	70,656	346,800
7	(57)	174,623	963,576
9	(59)	67,784	224,673
11	(61)	126,619	757,598
13	(63)	53,895	301,068
14	(63)	62,014	261,651
15	(63)	72,199	237,282
17	(65)	31,407	136,617
18	(65)	103,277	335,492
19	(65)	49,710	73,513
21	(10)	119,533	303,437
23	(12)	40,700	109,916
25	(11)	37,113	58,609
27	(85)	7,979	169,440
29	(87)	78,626	289,021
30	(87)	28,258	103,110
31	(87)	58,401	155,584
33	(89)	26,455	94,572
35	(91)	31,609	137,167
37	(93)	22,990	60,046
39	(95)	129,161	395,501
43	(97)	85,758	283,045
45	(99)	167,829	548,493
47	(101)	76,822	222,646
49	(105)	159,626	538,679
51	(2)	143,169	713,753
53	N	443,751	2,379,336
55	W	58,453	652,514
57	E	38,865	436,665
59	S	26,275	268,382



Signature... ....Page 58 of 103

Table 3 (continued). Halocarbons (abundance per sample as a percentage of the total abundance for samples 1 – 49)

Sample Number	Context Number	Dicholoromethane	Chloroform
1	(51)	3.64	3.48
3	(53)	2.69	3.28
5	(55)	3.51	4.55
7	(57)	8.69	12.64
9	(59)	3.37	2.95
11	(61)	6.30	9.94
13	(63)	2.68	3.95
14	(63)	3.08	3.43
15	(63)	3.59	3.11
17	(65)	1.56	1.79
18	(65)	5.14	4.40
19	(65)	2.47	0.96
21	(10)	5.96	3.98
23	(12)	2.02	1.44
25	(11)	1.85	0.76
27	(85)	0.40	2.22
29	(87)	3.91	3.79
30	(87)	1.41	1.35
31	(87)	2.90	2.04
33	(89)	1.32	1.24
35	(91)	1.57	1.80
37	(93)	1.14	0.79
39	(95)	6.42	5.19
43	(97)	4.27	3.71
45	(99)	8.35	7.20
47	(101)	3.82	2.92
49	(105)	7.94	7.07
51	(2)	7.12	9.36
53	N	22.07	31.22
55	W	2.91	8.56
57	E	1.93	5.73
59	S	1.31	3.52



Signature... Lorna Dawson ....Page 59 of 103

Table 3 (continued). Halocarbons.

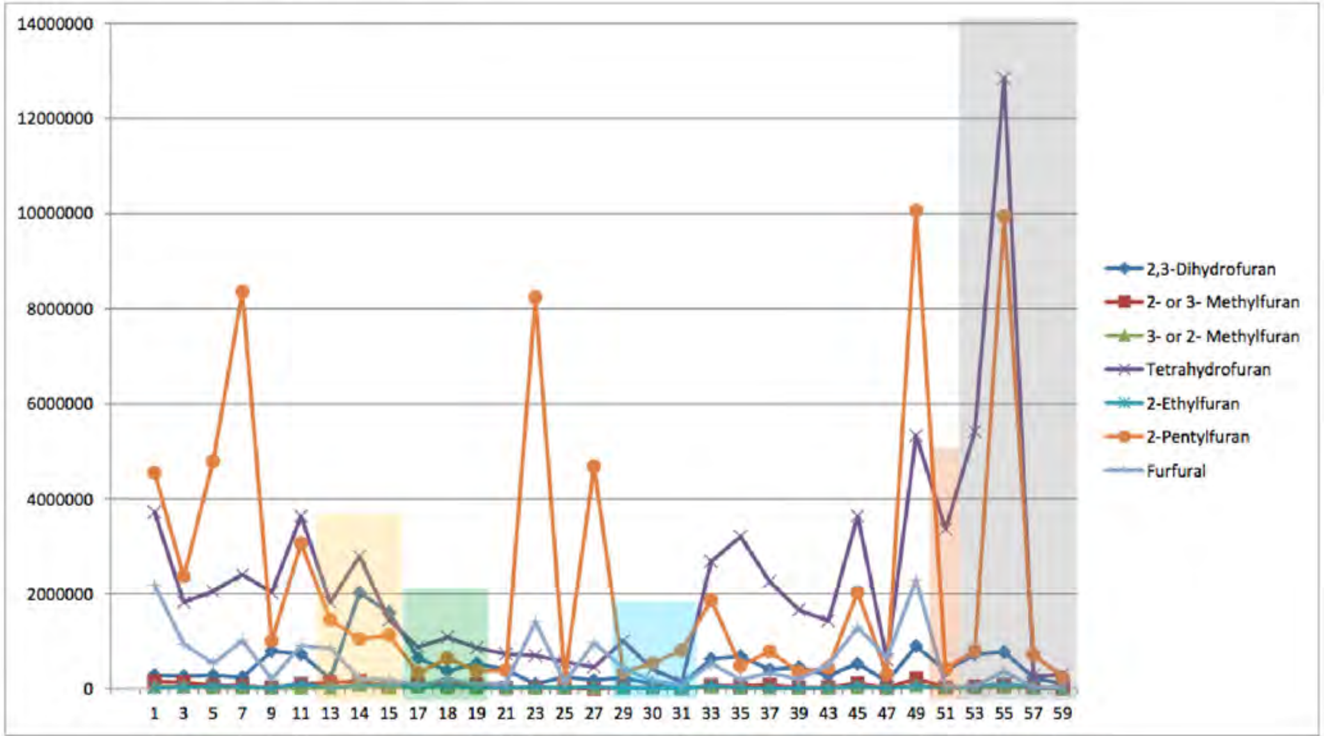
- Dichloromethane and chloroform were the only halocarbons detected in the samples.
- Abundance profiles for dichloromethane and chloroform were broadly similar across the samples, with abundance maxima for samples 7, 9 and an increase towards the western cells (higher sample numbers) and baulk sample (51) culminating with maximum abundance for the Northern boundary sample (53).
- Chloroform is a non-specific mammalian decomposition marker.

Table 3 (continued). Furans (abundance per g of sample)

Sample Number	Context Number	2,3-Dihydrofuran	2- or 3- Methylfuran	3- or 2- Methylfuran	Tetrahydrofuran	2-Ethylfuran	2-Pentylfuran	Furfural
1	(51)	288,592	155,496	48,906	3,719,482	21,677	4,550,141	2,185,563
3	(53)	270,860	140,241	50,897	1,824,967	36,429	2,363,064	944,200
5	(55)	290,260	69,999	29,315	2,054,782	58,265	4,786,625	534,534
7	(57)	245,171	68,889	28,157	2,403,880	47,551	8,358,903	1,019,374
9	(59)	799,620	26,231	17,516	2,029,268	24,941	1,008,343	203,673
11	(61)	731,868	100,981	20,293	3,633,090	114,077	3,058,884	912,742
13	(63)	215,930	134,194	15,987	1,822,136	19,221	1,457,231	856,072
14	(63)	2,023,583	165,340	88,715	2,789,230	67,589	1,047,524	217,682
15	(63)	1,614,248	62,914	28,289	1,444,939	85,423	1,132,652	193,502
17	(65)	647,873	93,534	53,385	875,088	35,539	338,449	82,111
18	(65)	377,568	85,297	27,514	1,090,671	61,171	648,572	201,127
19	(65)	536,092	84,237	18,480	861,625	27,165	378,055	103,802
21	(10)	403,861	21,322	11,888	732,884	30,846	391,989	120,175
23	(12)	102,680	31,135	13,995	702,125	49,345	8,242,337	1,415,124
25	(11)	259,069	24,004	31,062	565,404	21,569	229,400	144,109
27	(85)	183,440	0	35,430	460,265	49,787	4,679,686	964,882
29	(87)	240,413	34,714	18,308	1,007,528	17,623	348,899	432,944
30	(87)	104,629	21,810	18,273	414,501	16,290	538,215	166,818
31	(87)	89,014	12,447	16,289	146,000	12,765	814,730	88,866
33	(89)	632,193	70,629	43,300	2,683,212	71,326	1,872,179	529,104
35	(91)	686,501	62,979	25,636	3,203,905	27,010	483,851	198,098
37	(93)	407,684	84,927	17,128	2,258,439	15,278	789,990	337,945
39	(95)	456,315	29,631	14,478	1,662,278	17,239	356,204	204,137
43	(97)	284,907	33,910	16,968	1,433,063	17,195	443,553	505,107
45	(99)	528,193	115,082	36,694	3,637,091	68,550	2,032,095	1,297,643
47	(101)	158,073	21,193	16,912	608,892	12,721	306,523	656,824
49	(105)	903,491	220,074	74,227	5,330,329	60,083	10,056,635	2,299,799
51	(2)	384,100	33,344	16,127	3,364,463	19,201	431,271	53,600
53	N	728,054	50,690	23,179	5,420,177	47,457	802,369	57,388
55	V	777,980	77,890	40,968	12,849,976	112,156	3,947,694	369,780
57	E	234,662	22,817	14,780	270,592	26,479	726,062	27,671
59	S	107,586	16,949	7,533	296,644	19,862	238,194	44,801

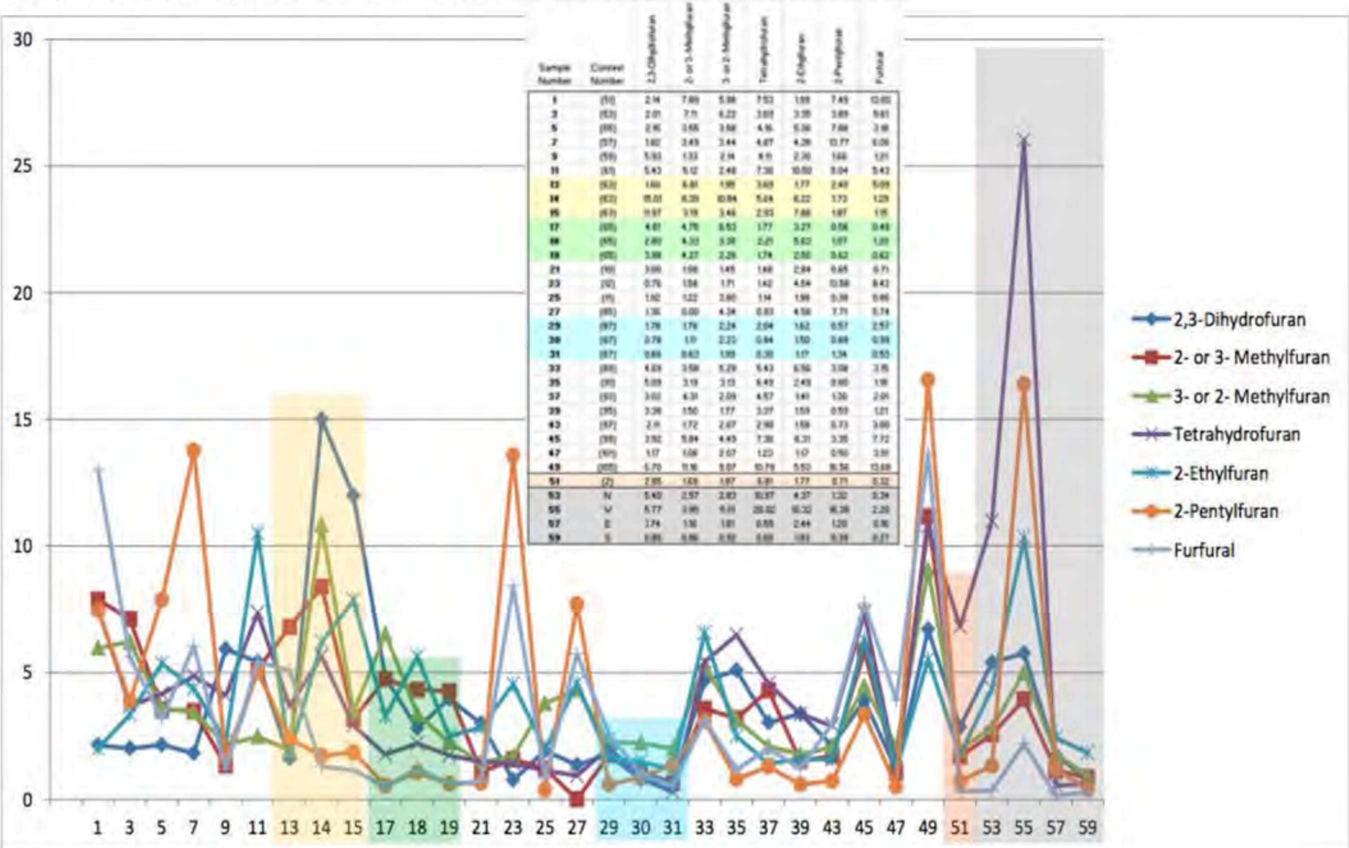
Signature... [signature] ....Page 61 of 103

Table 3 (continued). Furans (abundance per g of sample)



Signature... [signature] ....Page 62 of 103

Table 3 (continued). Furans (abundance per sample as a percentage of the total abundance for samples 1 – 49)



Signature... ....Page 63 of 103

Table 3 (continued). Furans

- A series of four alkyl substituted furans was found in the samples. Most of the compounds present were substituted at C-2 in the furan ring (2-methyl-, 2-ethyl- and 2-pentylfuran) and one at C-3 (3-methylfuran). Reduced (hydrogenated) furan derivatives, 2,3-dihydrofuran and tetrahydrofuran (THF) were also detected along with the aldehyde furfural (furan-2-carboxaldehyde).
- The most abundant furan derivatives were 2-pentyl furan with hotspots at samples 1-7, 11, 23, 27, 49 and the western boundary sample (55) and THF with hotspots at samples 1-15, 33-45, 49, baulk sample 51 and the Northern (53) and Western boundary samples (55). The distribution of the other furans follows a broadly similar pattern to a combination of those for 2-pentylfuran and THF.
- Furans, including 2-methyl furan and furans with other substituents are found in adult human and animal decomposition, but may not be expected (2-methyl furan) for children under 4 years old.

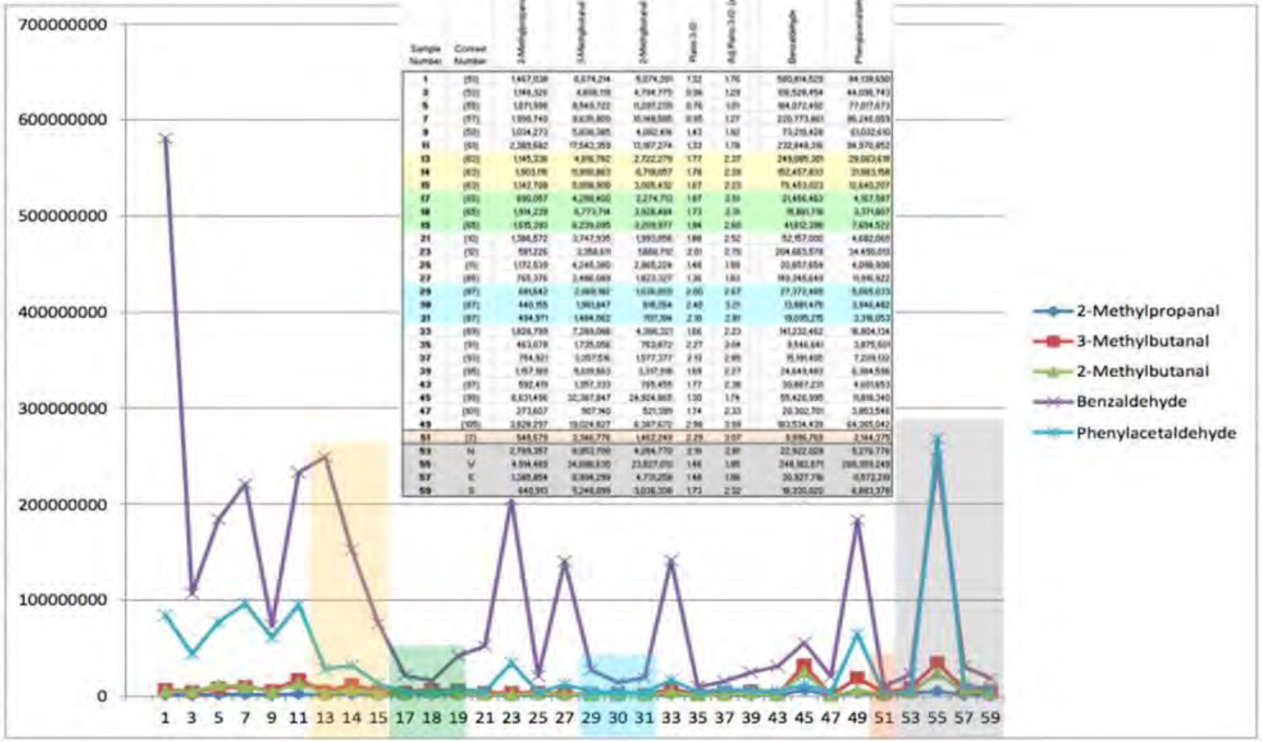
Table 3 (continued). Branched and aromatic aldehydes (abundance per g of sample)

Sample Number	Context Number	2-Methylpropanal	3-Methylbutanal	2-Methylbutanal	Ratio 3-/2-	Adj Ratio 3-/2- (x 1.34)	Benzaldehyde	Phenylacetaldehyde
1	(51)	1,467,038	6,674,214	5,074,201	1.32	1.76	580,814,529	84,139,690
3	(53)	1,148,326	4,606,119	4,794,775	0.96	1.29	106,528,454	44,096,743
5	(55)	1,871,998	8,549,722	11,297,239	0.76	1.01	184,072,492	77,017,673
7	(57)	1,990,740	9,635,800	10,148,585	0.95	1.27	220,773,861	96,246,059
9	(59)	1,034,273	5,838,385	4,082,414	1.43	1.92	73,219,428	61,032,610
11	(61)	2,389,682	17,543,359	13,187,274	1.33	1.78	232,848,316	94,970,852
13	(63)	1,145,336	4,816,782	2,722,279	1.77	2.37	249,085,301	28,063,618
14	(63)	1,903,116	11,990,863	6,719,057	1.78	2.39	152,457,833	31,863,158
15	(63)	1,142,708	5,008,900	3,005,432	1.67	2.23	75,453,023	12,640,207
17	(65)	890,057	4,258,400	2,274,713	1.87	2.51	21,456,463	4,167,587
18	(65)	1,914,239	6,773,714	3,926,484	1.73	2.31	15,881,718	3,371,807
19	(65)	1,615,393	6,239,095	3,209,977	1.94	2.60	41,812,398	7,694,522
21	(10)	1,386,572	3,747,935	1,993,056	1.88	2.52	52,157,000	4,682,060
23	(12)	581,226	3,359,611	1,668,712	2.01	2.70	204,663,578	34,490,013
25	(11)	1,172,539	4,245,380	2,865,224	1.48	1.99	20,857,654	4,098,908
27	(85)	765,376	2,486,089	1,823,327	1.36	1.83	140,345,649	11,916,922
29	(87)	681,642	2,068,182	1,036,059	2.00	2.67	27,372,465	5,065,033
30	(87)	440,155	1,961,847	818,264	2.40	3.21	13,881,475	3,946,482
31	(87)	494,971	1,484,062	707,194	2.10	2.81	19,095,215	3,316,053
33	(89)	1,828,799	7,289,088	4,386,321	1.66	2.23	141,232,462	16,804,134
35	(91)	463,078	1,735,056	763,872	2.27	3.04	9,546,641	3,875,501
37	(93)	754,921	3,357,516	1,577,377	2.13	2.85	15,191,405	7,209,132
39	(95)	1,157,189	5,619,563	3,317,918	1.69	2.27	24,649,483	6,384,596
43	(97)	592,419	1,357,333	765,455	1.77	2.38	30,867,231	4,601,653
45	(99)	6,631,496	32,387,847	24,924,865	1.30	1.74	55,426,995	11,818,340
47	(101)	273,607	907,140	521,399	1.74	2.33	20,302,701	3,853,546
49	(105)	3,828,297	19,024,827	6,367,672	2.98	3.99	183,534,439	64,365,042
51	(2)	548,679	3,346,776	1,462,249	2.29	3.07	9,996,769	2,144,375
53	N	2,789,357	8,953,700	4,264,770	2.10	2.81	22,922,029	5,276,776
55	V	4,914,489	34,686,630	23,827,013	1.46	1.95	248,182,671	268,359,249
57	E	1,385,854	6,994,299	4,731,258	1.48	1.98	30,927,716	11,572,219
59	S	640,913	5,248,099	3,036,338	1.73	2.32	18,330,022	6,883,378

Ta

Signature... *Lorna Dawson* ....Page 65 of 103

Table 3 (continued). Branched and aromatic aldehydes (abundance per g of sample)

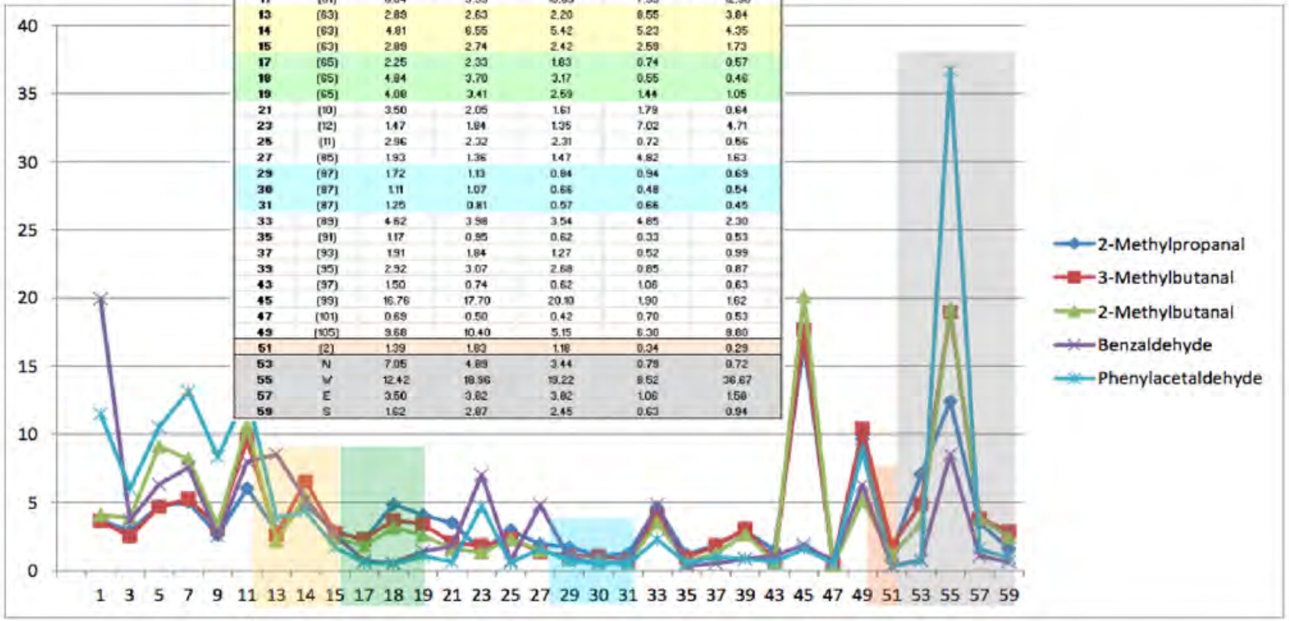


Sample Number	Context Number	2-Methylpropanal	3-Methylbutanal	2-Methylbutanal	Ratio 3:2	Adj Ratio 3:2 (x1.34)	Benzaldehyde	Phenylacetaldehyde
1	(51)	1,467,038	6,674,214	5,074,201	1.32	1.76	580,814,523	84,139,630
3	(53)	1,149,329	4,608,119	4,794,775	0.96	1.29	108,529,454	44,036,743
5	(55)	1,071,996	8,545,722	11,297,239	0.76	1.01	184,072,492	77,017,673
7	(57)	1,050,740	9,635,800	10,148,585	0.95	1.27	220,773,661	86,240,059
9	(59)	1,034,273	5,836,385	4,082,616	1.43	1.92	73,219,428	61,032,610
11	(61)	2,389,662	17,542,359	13,187,274	1.33	1.78	232,848,316	96,570,852
13	(62)	1,145,336	4,816,792	2,722,279	1.77	2.37	249,085,301	29,083,618
14	(63)	1,903,116	11,990,863	6,719,057	1.78	2.39	152,457,833	31,083,158
15	(63)	1,142,709	5,008,900	3,005,432	1.67	2.23	75,453,023	12,640,207
17	(65)	890,057	4,298,400	2,274,713	1.87	2.51	21,656,463	4,107,587
18	(65)	1,914,239	6,773,714	3,928,484	1.73	2.31	15,881,716	3,371,607
19	(65)	1,615,293	6,239,095	3,209,977	1.94	2.60	41,812,398	7,634,522
21	(70)	1,386,672	3,747,935	1,993,058	1.88	2.52	52,157,000	4,682,065
23	(70)	591,226	3,358,611	1,666,712	2.01	2.70	204,663,578	34,450,013
25	(71)	1,172,639	4,245,380	2,865,224	1.48	1.98	20,857,654	4,099,938
27	(85)	765,376	2,486,089	1,823,327	1.36	1.83	140,265,643	11,916,922
29	(87)	691,642	2,089,167	1,036,859	2.05	2.67	27,372,486	5,065,033
30	(87)	440,155	1,903,847	916,254	2.40	3.21	13,881,475	3,946,462
31	(87)	434,371	1,494,062	707,394	2.10	2.81	19,095,215	3,316,053
33	(89)	1,828,799	7,289,068	4,386,321	1.66	2.23	141,232,462	16,804,134
35	(91)	463,078	1,735,056	763,672	2.27	3.04	8,546,641	3,875,601
37	(93)	784,921	3,257,516	1,577,377	2.13	2.85	15,191,400	7,209,132
39	(95)	1,157,389	5,639,863	3,317,918	1.69	2.27	24,649,487	6,384,598
43	(97)	592,419	1,357,333	765,455	1.77	2.38	30,867,231	4,601,653
45	(99)	6,631,456	32,387,847	24,924,865	1.30	1.74	55,426,395	11,818,340
47	(101)	273,607	907,340	521,389	1.74	2.33	20,302,701	3,853,546
49	(105)	3,829,297	19,024,827	6,387,672	2.98	3.99	183,534,439	64,265,042
51	(7)	548,679	3,346,776	1,462,249	2.29	3.07	9,996,759	2,144,275
53	N	2,769,357	8,853,700	4,284,770	2.19	2.91	22,922,029	5,279,779
55	V	4,914,469	34,888,830	23,827,013	1.46	1.95	248,182,671	266,359,249
57	E	1,385,854	6,894,259	4,731,258	1.48	1.96	30,927,776	9,572,219
59	S	640,913	5,248,099	3,036,336	1.73	2.32	18,220,022	6,883,378

Signature... *[signature]* ....Page 66 of 103

Table 3 (continued). Branched and aromatic aldehydes (abundance per sample expressed as a percentage of the total abundance for samples 1 – 49)

Sample Number	Context Number	2-Methylpropanal	3-Methylbutanal	2-Methylbutanal	Benzaldehyde	Phenylacetaldehyde
1	(51)	3.71	3.65	4.09	19.94	11.50
3	(53)	2.90	2.52	3.87	3.66	6.03
5	(55)	4.73	4.67	9.11	6.32	10.53
7	(57)	5.03	5.27	8.18	7.58	13.15
9	(59)	2.61	3.19	3.29	2.51	8.34
11	(61)	6.04	9.59	10.63	7.99	12.98
13	(63)	2.89	2.63	2.20	8.55	3.84
14	(63)	4.81	6.55	5.42	5.23	4.35
15	(63)	2.89	2.74	2.42	2.59	1.73
17	(65)	2.25	2.33	1.83	0.74	0.57
18	(65)	4.84	3.70	3.17	0.55	0.46
19	(65)	4.08	3.41	2.59	1.44	1.05
21	(10)	3.50	2.05	1.61	1.79	0.64
23	(12)	1.47	1.84	1.35	7.02	4.71
25	(11)	2.96	2.32	2.31	0.72	0.86
27	(85)	1.93	1.36	1.47	4.82	1.63
29	(87)	1.72	1.13	0.84	0.94	0.69
30	(87)	1.11	1.07	0.66	0.48	0.54
31	(87)	1.25	0.81	0.57	0.66	0.45
33	(89)	4.62	3.98	3.54	4.85	2.30
35	(91)	1.17	0.95	0.62	0.33	0.53
37	(93)	1.91	1.84	1.27	0.52	0.99
39	(95)	2.92	3.07	2.68	0.85	0.87
43	(97)	1.50	0.74	0.62	1.06	0.63
45	(99)	16.76	17.70	20.10	1.90	1.62
47	(101)	0.69	0.50	0.42	0.70	0.53
49	(105)	9.68	10.40	5.15	6.30	8.80
51	(2)	1.39	1.83	1.18	0.34	0.29
53	N	7.05	4.89	3.44	0.79	0.72
55	W	12.42	18.96	19.22	8.52	36.67
57	E	3.50	3.82	3.82	1.06	1.58
59	S	1.62	2.87	2.45	0.63	0.94



Signature... *[signature]* ....Page 67 of 103

Table 3 (continued). Branched and aromatic aldehydes

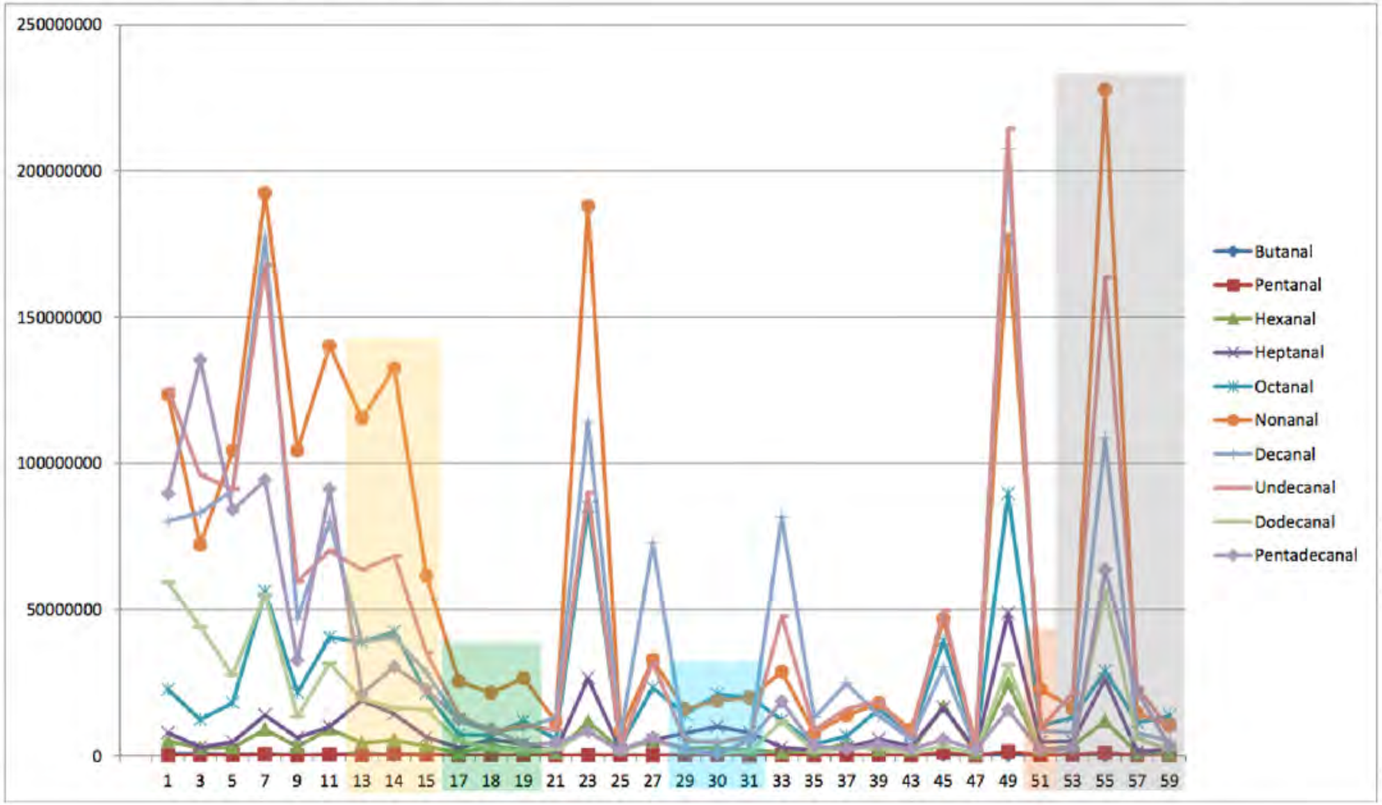
- The three short chain branched aldehydes, 2-methylpropanal, 3-methylbutanal and 2-methyl butanal were detected in all samples with 3-/2- isomer ratios in the range of 1.27 – 3.07 for all but one sample (5) which had an isomer ratio 1.01. These isomer ratios are consistent with a human decomposition process.
- The br-aldehydes were most abundant for samples 5, 7, 11, 14, 45 and 49, and for the Western boundary sample (55).
- Benzaldehyde and phenylacetaldehyde were found in the samples, with broadly similar abundance profiles. Abundance maxima were seen for samples 1-9, 11-15, 23, 27, 33, 49, and for the Western boundary sample (55).

Table 3 (continued). *n*-Aldehydes (abundance per g of sample)

Sample Number	Context Number	Butanal	Pentanal	Hexanal	Heptanal	Octanal	Nonanal	Decanal	Undecanal	Dodecanal	Pentadecanal
1	(51)	715,924	117,323	5,138,056	7,837,787	22,580,981	123,418,467	80,195,249	125,432,351	59,222,029	89,622,683
3	(53)	690,399	213,551	2,611,780	2,863,722	12,298,452	72,121,688	83,117,050	95,929,277	44,138,752	135,224,895
5	(55)	316,920	259,478	2,819,138	4,665,118	18,063,540	104,296,128	90,766,921	91,244,182	27,563,649	83,988,562
7	(57)	396,977	433,690	8,983,526	13,888,887	56,086,838	192,378,078	177,449,617	167,807,913	55,184,025	94,249,323
9	(59)	85,586	72,103	3,124,577	6,079,850	21,544,332	104,321,020	46,821,768	59,577,522	13,375,746	32,556,574
11	(61)	150,408	417,738	9,181,875	9,925,577	40,440,765	140,117,841	80,065,707	70,125,143	31,611,556	91,087,884
13	(63)	877,606	153,597	4,380,025	18,997,632	38,894,665	115,346,020	38,925,991	63,586,177	19,397,591	21,119,828
14	(63)	199,430	545,832	5,365,876	14,252,609	42,400,034	132,500,370	40,427,460	68,275,277	18,423,793	30,338,107
15	(63)	124,636	325,316	3,284,389	6,301,824	21,357,680	61,554,210	28,415,716	35,160,131	15,813,979	22,682,596
17	(65)	46,930	106,684	999,406	2,700,385	7,179,363	25,395,321	11,879,387	14,004,080	5,042,933	12,345,600
18	(65)	87,203	141,807	3,370,522	5,596,688	6,919,517	21,473,207	6,247,266	7,916,270	2,615,599	9,228,779
19	(65)	59,121	191,168	2,089,612	4,045,703	11,850,805	26,493,968	9,378,193	10,475,393	1,726,204	3,844,191
21	(10)	43,568	81,397	1,062,049	1,809,046	5,601,585	11,631,482	13,064,051	8,843,993	2,306,295	4,320,568
23	(12)	75,588	197,345	11,726,772	26,525,456	85,080,418	187,918,791	114,248,567	90,071,849	8,720,722	8,160,172
25	(11)	56,768	212,013	2,053,503	1,977,905	3,339,016	8,313,037	6,633,023	2,824,213	1,190,403	1,879,166
27	(85)	32,928	62,371	5,076,219	5,414,064	23,214,813	32,814,383	72,719,125	32,044,350	5,503,247	6,172,155
29	(87)	43,805	267,346	2,745,241	7,886,233	14,230,910	15,930,785	4,958,924	5,155,947	1,434,719	2,152,801
30	(87)	41,640	231,121	2,605,441	9,974,221	20,941,170	18,776,716	4,861,034	4,596,873	660,765	619,067
31	(87)	19,762	49,015	2,002,685	7,889,740	20,087,818	19,837,284	5,960,185	6,625,722	1,563,805	5,401,508
33	(89)	119,087	130,188	1,045,775	2,819,649	12,132,813	28,705,826	81,596,059	47,808,058	11,765,070	18,530,505
35	(91)	69,177	98,760	1,801,181	1,933,560	3,897,570	7,813,656	13,023,561	8,731,389	1,492,435	3,454,110
37	(93)	49,826	189,899	4,036,468	2,730,595	6,651,617	13,761,003	24,757,507	16,051,252	2,584,172	2,200,233
39	(95)	49,417	204,176	2,049,450	5,630,551	15,916,435	17,947,754	13,622,577	18,583,441	2,754,632	3,948,959
43	(97)	34,031	67,413	1,872,070	3,251,635	6,992,009	8,883,282	5,595,300	6,685,251	966,186	2,290,577
45	(99)	157,452	1,037,409	16,761,305	16,354,642	39,241,253	46,719,433	30,209,594	49,681,958	3,304,265	5,627,983
47	(101)	17,816	25,455	929,031	1,996,274	3,864,720	3,777,380	2,386,851	2,307,533	741,766	2,034,229
49	(105)	171,364	1,425,338	24,696,123	48,772,361	89,632,901	176,524,823	207,419,703	214,380,446	31,023,271	15,761,048
51	(2)	33,467	152,751	2,004,420	4,697,341	10,196,998	22,681,178	8,376,895	9,348,190	1,314,602	1,878,519
53	N	98,224	299,830	3,351,362	4,930,283	13,087,187	16,381,648	8,111,499	21,444,678	2,789,613	2,623,005
55	W	77,121	1,039,213	11,890,520	26,131,432	28,917,033	227,814,185	108,560,980	163,851,432	56,483,900	63,595,020
57	E	32,844	68,889	907,892	1,274,898	11,267,385	14,525,581	7,752,250	23,157,259	5,917,621	21,908,928
59	S	34,754	53,929	698,385	2,236,629	13,644,687	10,229,449	5,152,875	9,269,047	2,167,451	3,274,050

Signature... [signature] ....Page 69 of 103

Table 3 (continued). *n*-Aldehydes (abundance per g of sample)



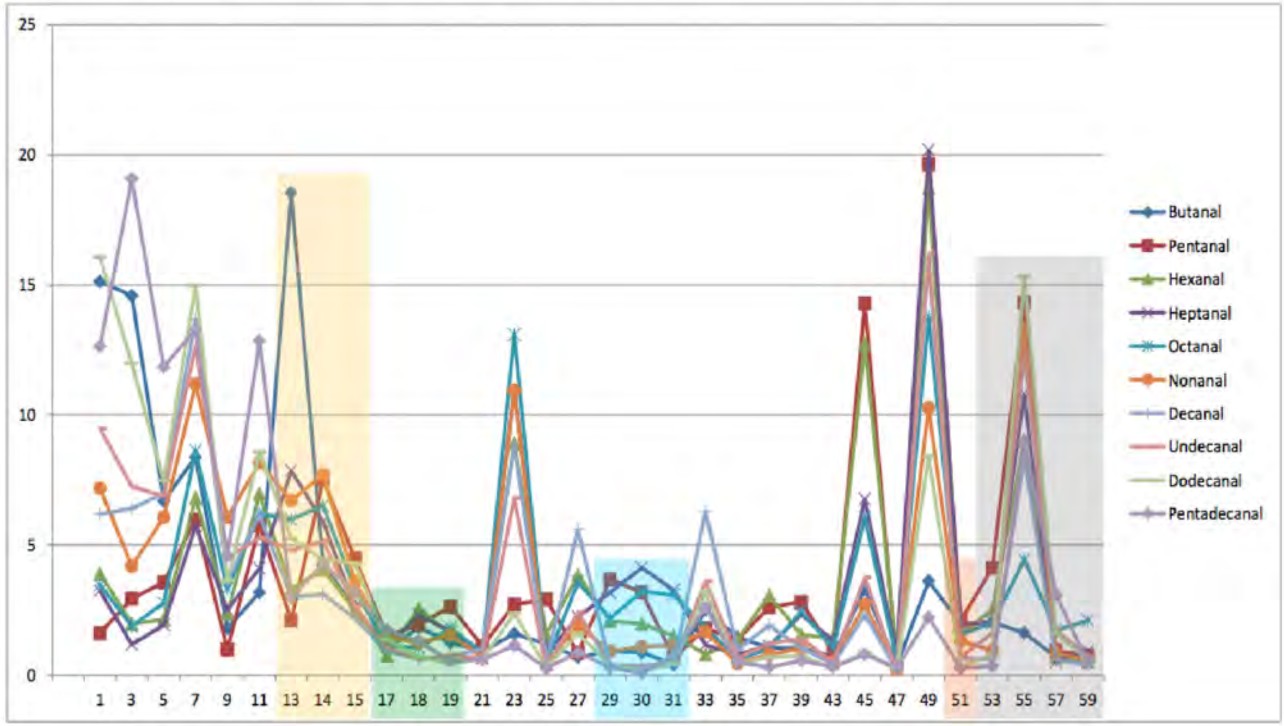
Signature... ....Page 70 of 103

Table 3 (continued). *n*-Aldehydes (abundance per sample as a percentage of the total abundance for samples 1 – 49)

Sample Number	Context Number	Butanal	Pentanal	Hexanal	Heptanal	Octanal	Nonanal	Decanal	Undecanal	Dodecanal	Pentadecanal
1	(51)	15.13	1.62	3.90	3.24	3.47	7.18	6.19	9.48	16.07	12.64
3	(53)	14.59	2.94	1.98	1.18	1.89	4.20	6.41	7.25	11.98	19.08
5	(55)	6.70	3.57	2.14	1.93	2.76	6.07	7.00	6.89	7.48	11.85
7	(57)	8.39	5.97	6.82	5.75	8.62	11.19	13.69	12.68	14.97	13.30
9	(59)	1.61	0.99	2.37	2.52	3.31	6.07	3.61	4.50	3.63	4.59
11	(61)	3.18	5.75	6.97	4.11	6.22	8.15	6.18	5.30	8.58	12.85
13	(63)	18.54	2.12	3.31	7.86	5.98	6.71	3.00	4.80	5.26	2.98
14	(63)	4.21	7.52	4.07	5.90	6.52	7.71	3.12	5.16	4.46	4.28
15	(63)	2.63	4.48	2.49	2.61	3.28	3.58	2.19	2.66	4.29	3.20
17	(65)	0.99	1.50	0.76	1.12	1.10	1.48	0.92	1.06	1.37	1.74
18	(65)	1.84	1.95	2.56	2.32	1.06	1.25	0.64	0.60	0.71	1.30
19	(65)	1.25	2.63	1.59	1.67	1.82	1.54	0.72	0.79	0.47	0.54
21	(10)	0.92	1.12	0.81	0.67	0.86	0.68	1.01	0.65	0.63	0.61
23	(12)	1.60	2.72	8.90	10.97	13.08	10.93	8.81	6.80	2.37	1.15
25	(11)	1.20	2.92	1.56	0.82	0.51	0.48	0.51	0.21	0.32	0.27
27	(85)	0.70	0.86	3.85	2.24	3.57	1.91	5.61	2.42	1.60	0.87
29	(87)	0.93	3.68	2.08	3.18	2.19	0.93	0.38	0.39	0.39	0.30
30	(87)	0.88	3.18	1.98	4.13	3.22	1.09	0.36	0.35	0.18	0.09
31	(87)	0.42	0.68	1.52	3.26	3.09	1.15	0.46	0.50	0.42	0.76
33	(89)	2.52	1.79	0.79	1.17	1.87	1.67	6.29	3.61	3.19	2.61
35	(91)	1.46	1.36	1.37	0.80	0.60	0.45	1.00	0.66	0.40	0.49
37	(93)	1.05	2.62	3.06	1.13	1.02	0.80	1.91	1.21	0.70	0.31
39	(95)	1.04	2.81	1.56	2.33	2.45	1.04	1.05	1.40	0.75	0.56
43	(97)	0.72	0.93	1.42	1.35	1.07	0.52	0.43	0.51	0.26	0.32
45	(99)	3.33	14.29	12.72	6.77	6.03	2.72	2.33	3.75	0.90	0.79
47	(101)	0.38	0.35	0.70	0.83	0.59	0.22	0.18	0.17	0.20	0.29
49	(105)	3.62	19.63	18.74	20.18	13.78	10.27	16.00	16.20	8.42	2.22
51	(2)	1.97	2.10	1.52	1.94	1.57	1.32	0.65	0.71	0.36	0.27
53	N	2.03	4.13	2.54	2.04	2.01	0.95	0.63	1.62	0.76	0.37
55	W	1.63	14.32	5.02	10.81	4.45	13.25	8.37	12.36	15.33	8.97
57	E	0.69	0.95	0.69	0.53	1.73	0.85	0.60	1.75	1.61	3.09
59	S	0.73	0.74	0.52	0.93	2.10	0.60	0.40	0.70	0.59	0.46

Signature... ....Page 71 of 103

Table 3 (continued). *n*-Aldehydes (abundance per sample as a percentage of the total abundance for samples 1 – 49)



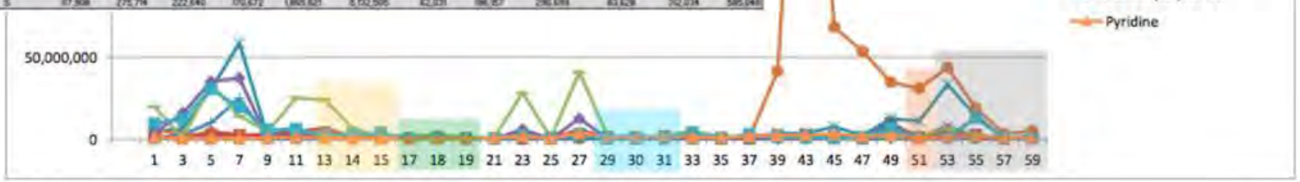
Signature... ....Page 72 of 103

Table 3 (continued). *n*-Aldehydes

- Ten aldehydes of this type were detected in the samples including butanal (C_4), pentanal (C_5), hexanal (C_6), heptanal (C_7), octanal (C_8), nonanal (C_9), decanal (C_{10}) undecanal (C_{11}) and pentadecanal (C_{15}).
- Of these the C_8-C_{11} aldehydes, octanal, nonanal, decanal, and unecanal were the most abundant homologues with abundance maxima for samples 1-15, 23, 27, 33, 45 and 49, and for the Western boundary sample (55).
- Nonanal (C_9) and decanal (C_{10}) are considered of significance for burial decomposition of bone.

Table 3 (continued). Aromatic hydrocarbons (abundance per g of sample)

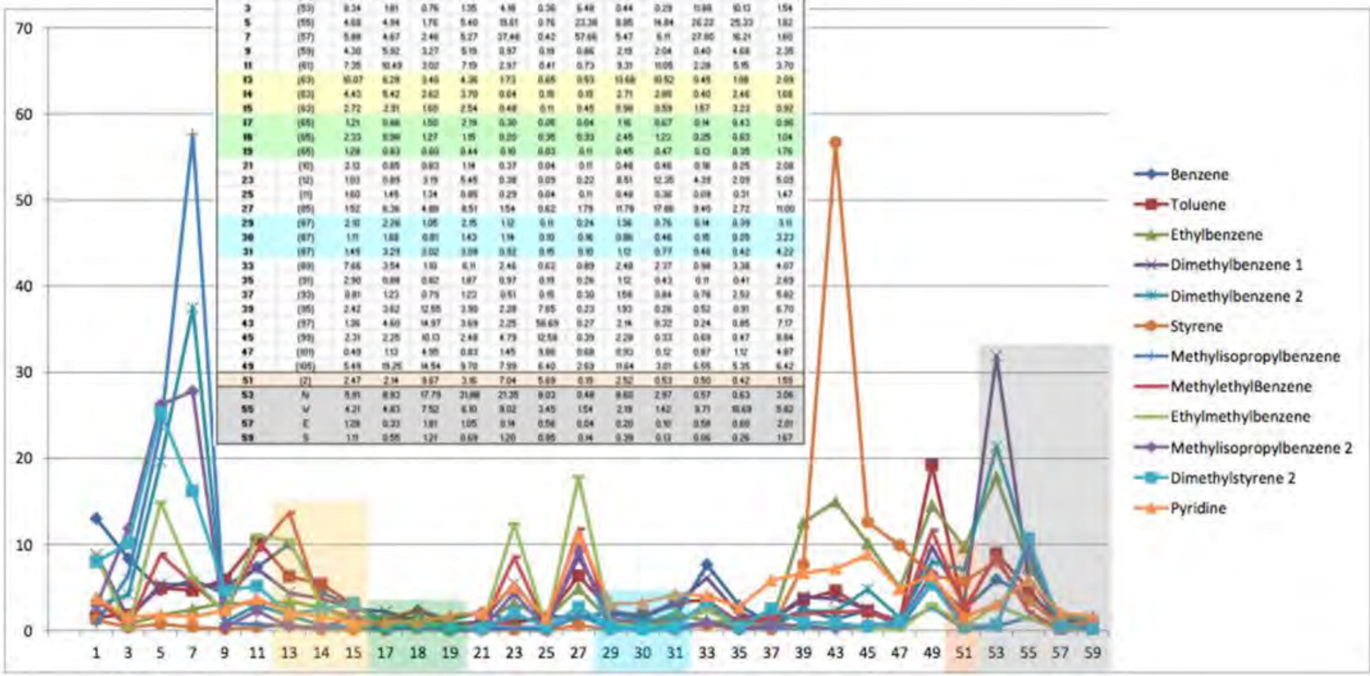
Sample Number	Context Number	Benzene	Toluene	Ethylbenzene	Dimethylbenzene 1	Dimethylbenzene 2	Styrene	Methylisopropylbenzene	Methylethylbenzene	Ethylmethylbenzene	Methylisopropylbenzene 2	Dimethylstyrene 2	Pyridine
1	(59)	1,279,904	794,807	834,651	2,983,004	4,501,037	6,770,490	340,249	1,810,344	19,643,839	3,971,456	5,045,829	1,309,062
3	(52)	886,229	303,799	139,667	324,353	6,503,919	1,930,046	2,790,522	217,472	667,811	15,893,677	12,224,672	529,389
5	(55)	497,354	2,470,647	323,916	1,329,885	30,550,183	4,145,072	10,070,766	4,412,653	33,840,686	35,072,772	30,556,340	636,994
7	(57)	624,340	2,333,537	451,654	1,308,763	58,374,271	2,262,532	24,832,746	2,724,568	13,927,778	37,183,632	19,549,616	560,112
9	(58)	456,356	2,960,595	600,328	1,288,154	1,512,272	1,040,637	270,372	1,089,619	4,657,560	532,823	5,643,805	821,141
11	(61)	780,329	5,245,809	555,703	1,794,867	4,624,230	2,230,804	312,932	4,641,780	25,139,118	3,054,757	6,215,151	1,294,263
13	(63)	1,869,732	3,143,054	825,283	1,082,155	2,691,259	3,522,688	227,456	6,817,960	23,989,654	595,706	2,285,894	730,795
14	(63)	470,445	2,712,388	480,671	917,160	389,259	794,611	63,930	1,349,416	6,490,990	532,516	2,963,620	588,877
15	(63)	288,554	1,458,985	293,408	629,414	747,220	575,851	192,105	488,062	1,346,349	2,093,886	3,893,365	322,294
17	(65)	128,323	439,029	274,754	542,505	472,704	258,310	19,275	577,175	1,525,916	188,509	513,240	335,293
18	(65)	247,509	490,852	234,231	295,332	307,156	1,902,029	140,898	1,221,679	2,807,770	329,590	760,849	362,556
19	(65)	136,450	413,422	109,924	169,630	155,518	162,187	45,960	221,858	1,074,290	180,216	418,850	616,503
21	(19)	225,977	426,626	152,073	282,958	573,180	218,112	45,462	236,717	1,044,482	237,445	303,103	728,814
23	(12)	109,777	443,060	596,217	1,353,334	593,599	505,213	95,557	4,242,738	28,168,862	5,873,978	2,526,459	1,779,892
25	(71)	170,270	723,197	246,548	211,485	448,649	211,591	48,834	236,758	829,712	115,036	378,748	514,134
27	(85)	61,268	2,182,096	697,368	2,111,309	2,391,884	3,353,911	771,862	5,869,179	40,710,471	12,573,825	3,276,724	3,847,113
29	(87)	222,835	1,127,945	182,324	532,654	1,750,623	595,033	104,908	677,072	1,729,515	183,947	479,363	1,085,893
30	(87)	119,239	839,107	148,372	354,192	1,792,135	535,694	66,988	430,876	1,040,283	206,064	200,259	1,129,884
31	(87)	157,756	1,647,280	370,612	767,587	1,425,589	900,845	43,855	555,909	1,757,085	613,864	512,591	1,476,798
33	(89)	913,823	1,770,346	201,721	1,516,156	3,827,757	3,362,882	384,866	1,239,072	5,411,212	1,309,759	4,074,948	1,423,798
35	(91)	307,630	439,796	150,956	463,250	1,512,480	1,028,863	113,431	598,111	939,778	147,405	492,450	940,155
37	(93)	86,269	514,596	144,917	306,295	789,814	818,634	127,643	785,139	1,520,924	1,038,990	3,044,104	2,033,316
39	(95)	256,794	1,809,172	2,305,643	969,031	3,548,264	41,673,766	99,077	963,049	603,815	700,969	1,103,157	2,342,118
43	(97)	144,261	2,299,301	2,750,270	914,576	3,504,511	307,535,307	117,768	1,068,959	732,156	323,039	1,019,890	2,506,091
45	(99)	245,844	1,125,668	1,891,073	614,922	7,461,869	68,219,544	168,844	1,137,632	762,409	923,779	561,913	3,088,643
47	(101)	52,259	563,053	909,305	206,972	2,262,730	53,462,112	293,166	465,312	270,534	1,168,845	1,351,008	1,701,845
49	(105)	580,029	9,629,505	2,470,651	2,406,924	12,439,864	24,727,305	1,159,286	5,799,122	6,860,361	6,767,554	6,448,715	2,245,298
51	(Z)	262,433	1,071,871	1,775,783	784,180	10,905,454	30,863,922	82,738	1,257,730	1,290,615	672,881	511,122	954,164
53	N	627,676	4,468,157	3,258,347	7,311,844	33,294,455	43,586,573	205,642	4,298,381	6,761,542	767,019	759,664	1,069,932
55	V	446,705	2,417,555	1,302,050	1,514,261	14,055,504	16,741,592	663,307	1,089,428	3,245,907	12,566,552	12,891,354	2,035,972
57	E	136,354	163,403	232,761	259,524	217,480	3,085,338	15,458	97,917	220,168	779,374	727,679	792,792
59	S	87,908	275,714	222,640	170,672	1,865,821	8,132,505	42,031	96,157	290,689	83,628	312,034	585,048



Signature... *[signature]* ....Page 74 of 103

Table 3 (continued). Aromatic hydrocarbons (abundance per sample as a percentage of the total abundance for samples 1 – 49)

Sample Number	Context Number	Benzene	Toluene	Ethylbenzene	Dimethylbenzene 1	Dimethylbenzene 2	Styrene	Methylisopropylbenzene	MethylethylBenzene	Ethylmethylbenzene	Methylisopropylbenzene 2	Dimethylstyrene 2	Pyridine
1	(51)	12.99	1.59	3.79	6.60	2.89	1.25	0.79	3.63	9.62	2.94	8.06	3.74
3	(53)	8.34	1.81	0.76	1.35	4.16	0.36	6.48	0.44	0.29	11.86	10.13	1.54
5	(55)	4.68	4.94	1.76	5.40	15.61	0.76	23.38	0.85	14.84	26.22	25.33	1.82
7	(57)	5.88	4.67	2.46	5.27	37.46	0.42	57.66	5.47	5.11	27.80	16.21	1.60
9	(59)	4.30	5.92	3.27	5.19	0.97	0.19	0.86	2.19	2.04	0.40	4.68	2.35
11	(61)	7.35	10.49	3.02	7.19	2.97	0.41	0.73	3.31	11.05	2.28	5.15	3.70
13	(63)	10.07	6.29	3.40	4.36	1.73	0.65	0.53	13.68	10.52	0.45	1.08	2.09
14	(63)	4.43	5.42	2.62	3.70	0.64	0.18	0.18	2.71	2.88	0.40	2.46	1.68
15	(63)	2.72	2.91	1.60	2.54	0.48	0.11	0.45	0.98	0.59	1.57	3.23	0.92
17	(65)	1.21	0.88	1.50	2.19	0.30	0.06	0.04	1.16	0.67	0.14	0.43	0.96
18	(65)	2.33	0.98	1.27	1.15	0.20	0.35	0.33	2.45	1.23	0.25	0.63	1.04
19	(65)	1.29	0.83	0.60	0.44	0.10	0.03	0.11	0.45	0.47	0.13	0.35	1.76
21	(10)	2.13	0.85	0.83	1.14	0.37	0.04	0.11	0.46	0.46	0.18	0.25	2.08
23	(12)	1.03	0.89	3.19	5.45	0.38	0.09	0.22	8.51	12.35	4.39	2.09	5.03
25	(11)	1.60	1.45	1.34	0.85	0.29	0.04	0.11	0.49	0.36	0.08	0.31	1.47
27	(85)	1.52	6.36	4.88	8.51	1.54	0.62	1.79	11.79	17.68	3.40	2.72	11.00
29	(87)	2.10	2.26	1.05	2.15	1.12	0.11	0.24	1.36	0.76	0.14	0.39	3.11
30	(87)	1.11	1.68	0.81	1.43	1.14	0.10	0.16	0.86	0.46	0.15	0.25	3.23
31	(87)	1.49	3.29	2.02	3.08	0.52	0.15	0.10	1.12	0.77	0.46	0.42	4.22
33	(89)	7.66	3.54	1.10	6.11	2.46	0.62	0.89	2.48	2.37	0.98	3.38	4.07
35	(91)	2.90	0.88	0.62	1.87	0.97	0.19	0.26	1.12	0.43	0.11	0.41	2.69
37	(93)	0.81	1.23	0.75	1.23	0.51	0.15	0.30	1.56	0.84	0.76	2.52	5.62
39	(95)	2.42	3.62	12.55	3.90	2.28	7.65	0.23	1.93	0.26	0.52	0.91	6.70
43	(97)	1.36	4.60	14.97	3.69	2.25	56.69	0.27	2.16	0.32	0.24	0.85	7.17
45	(99)	2.31	2.25	10.13	2.48	4.79	12.58	0.39	2.29	0.33	0.69	0.47	8.84
47	(101)	0.49	1.13	4.95	0.83	1.45	9.86	0.68	0.93	0.12	0.87	1.12	4.87
49	(105)	5.49	19.25	14.54	9.70	7.99	6.40	2.63	11.64	3.01	6.55	5.35	6.42
51	(2)	2.47	2.14	9.67	3.16	7.04	5.69	0.19	2.52	0.53	0.50	0.42	1.59
53	N	5.91	8.93	17.79	31.88	21.35	9.03	0.48	8.60	2.97	0.57	0.63	3.06
55	V	4.21	4.83	7.52	6.10	9.02	3.45	1.54	2.19	1.42	9.71	10.69	5.62
57	E	1.29	0.33	1.81	1.05	0.14	0.56	0.04	0.20	0.10	0.58	0.80	2.01
59	S	1.11	0.55	1.21	0.69	1.20	0.95	0.14	0.39	0.13	0.06	0.26	1.67



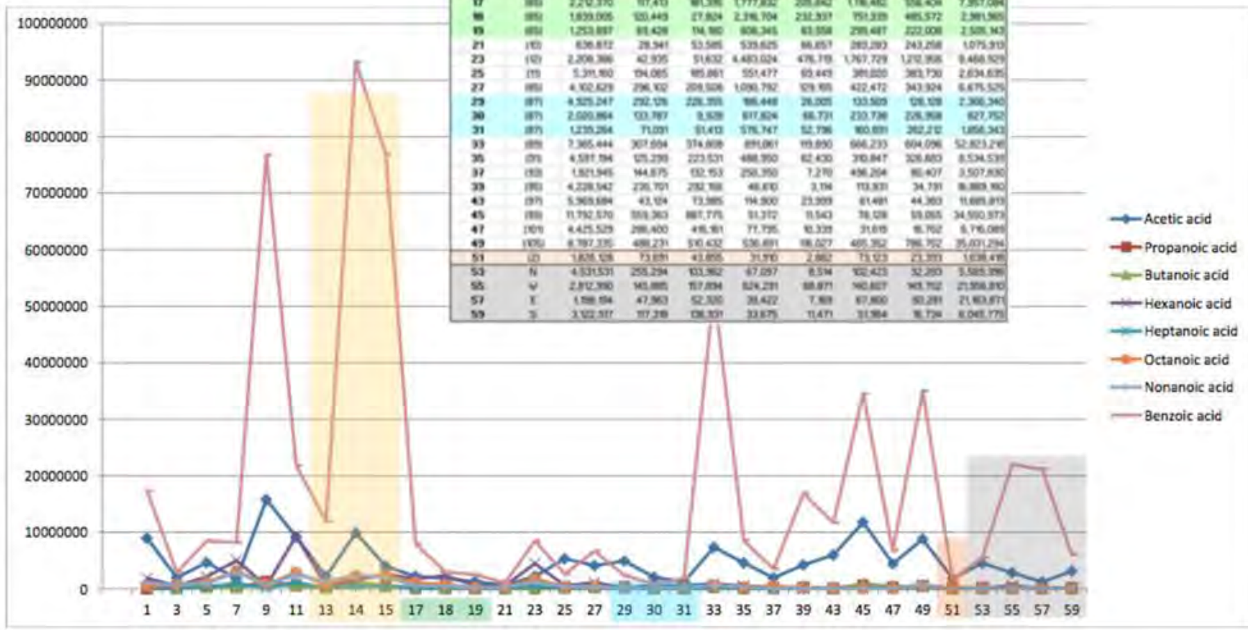
Signature... [signature] ....Page 75 of 103

Table 3 (continued). Aromatic hydrocarbons

- Eleven members of this class of compound, including benzene, toluene, ethyl benzene, ethylmethyl benzene, styrene, dimethyl styrene (or ethyl styrene), and multiple isomers of dimethyl benzene and methylisopropy benzene (or diethyl benzene) were detected in the samples. In addition the aromatic nitrogen-containing heterocyclic compound pyridine was detected.
- Abundance maxima for aromatic compounds were seen for samples 5, 7, 11, 13, 23, 27, 39 - 45 and 49, and for the Northern boundary sample (53). Interestingly, there is a shift in the dominant aromatics present in the samples when moving from eastern to western cells (low to high sample numbers). The methylisopropylbenzenes and one of the dimethylbenzenes (or ethylbenzene) dominate the distribution for samples 5 and 7, whereas the methylethyl/ethymethyl benzenes dominate for samples 11, 13, 23 and 27. Styrene and ethylbenzene (or dimethylbenzene) dominate at sample 43 and toluene and ethylbenzene (or dimethylbenzene) dominate at sample 49. The dimethylbenzenes/ethylbenzene and toluene dominate in the Northern boundary sample (53).
- Pyridine shows abundance maxima at samples 23, 27, 37-49 and the Western boundary sample (55).
- Benzene, toluene (methyl benzene), isomers of dimethyl benzene (xylenes), ethy methyl benzene and styrene (ethenyl benzene) are associated with mammalian decomposition but are considered to be non-specific.

Table 3 (continued). Carboxylic acids (abundance per g of sample)

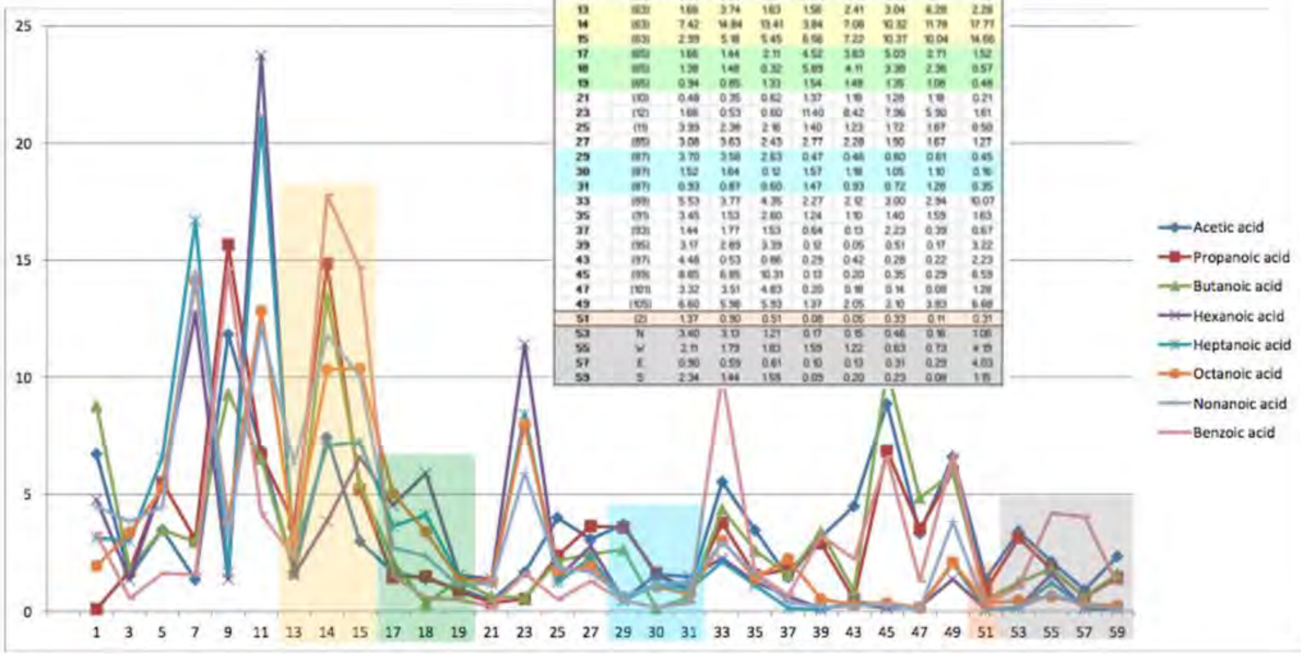
Sample Number	Context Number	Acetic acid	Propanoic acid	Butanoic acid	Hexanoic acid	Heptanoic acid	Octanoic acid	Nonanoic acid	Benzoic acid
1	(57)	8,337,494	7,760	756,142	1,865,551	177,471	429,636	321,240	17,362,324
3	(53)	1,399,310	136,309	164,856	529,794	183,974	743,913	798,832	2,870,596
5	(55)	4,633,242	449,250	295,481	2,135,460	372,098	1,161,697	515,392	8,463,679
7	(57)	1,802,712	249,776	254,078	5,008,234	344,633	3,137,320	2,973,155	8,177,246
9	(59)	15,745,250	1,277,384	790,542	535,596	94,170	843,877	688,439	76,741,082
11	(61)	3,174,871	545,007	580,416	9,332,082	1,194,330	2,848,836	2,438,009	21,811,004
13	(63)	2,206,679	305,377	140,098	612,269	136,622	674,895	1,289,679	11,937,252
14	(63)	9,887,600	1,211,751	1,154,537	1,511,788	401,032	2,293,015	2,421,321	93,231,155
15	(63)	3,976,633	422,703	469,494	2,381,361	408,633	2,302,486	2,063,014	76,894,246
17	(65)	2,212,370	117,413	181,395	1,777,832	205,842	1,176,482	556,404	7,357,084
18	(65)	1,839,005	120,449	27,824	2,316,704	232,337	751,339	485,572	2,381,365
19	(65)	1,253,897	93,428	114,160	808,345	63,558	299,487	222,008	2,505,143
21	(10)	636,872	28,341	53,585	539,625	86,857	283,283	243,258	1,075,913
23	(12)	2,208,386	42,935	51,632	4,483,024	476,719	1,767,729	1,212,958	9,468,929
25	(11)	5,311,160	194,085	185,861	551,477	93,443	381,020	383,730	2,634,635
27	(85)	4,102,629	296,102	209,506	1,090,792	129,155	422,472	343,924	6,675,525
29	(87)	4,525,247	292,126	228,355	186,448	26,005	133,509	128,128	2,366,340
30	(87)	2,020,864	133,787	9,939	617,824	66,731	233,736	226,958	627,752
31	(87)	1,235,264	71,031	51,413	576,747	52,796	160,691	262,212	1,856,343
33	(89)	7,365,444	307,694	374,608	891,061	119,850	666,233	604,096	52,823,216
35	(71)	4,591,194	125,290	223,531	488,350	62,430	310,847	326,603	8,534,535
37	(93)	1,921,945	144,875	132,153	250,350	7,270	436,204	80,407	3,507,830
39	(95)	4,228,542	230,701	232,168	46,610	3,114	113,931	34,791	16,869,160
43	(97)	5,969,684	43,124	73,985	114,900	23,939	61,481	44,363	11,685,813
45	(99)	11,792,570	559,363	887,775	51,372	11,543	78,128	59,065	34,550,973
47	(101)	4,425,529	288,400	416,161	77,795	10,339	31,615	16,702	6,716,085
49	(105)	8,787,335	488,231	510,432	536,691	116,027	485,352	786,752	35,031,294
51	(D)	1,826,126	73,691	43,855	31,310	2,862	73,123	23,313	1,638,416
53	N	4,531,531	255,294	103,362	67,097	8,514	102,423	32,250	5,585,396
55	V	2,812,390	145,885	157,894	824,291	88,871	140,607	145,752	21,958,810
57	E	1,198,194	47,963	52,320	28,422	7,169	67,800	90,281	21,163,871
59	S	3,122,517	117,218	136,331	33,675	11,471	31,984	16,734	6,045,775



Signature... ....Page 77 of 103

Table 3 (continued). Carboxylic acids (abundance per sample as a percentage of the total abundance for samples 1 – 49)

Sample Number	Context Number	Acetic acid	Propanoic acid	Butanoic acid	Hexanoic acid	Heptanoic acid	Octanoic acid	Nonanoic acid	Benzoic acid
1	(51)	6.71	0.10	8.78	4.75	3.13	1.93	4.48	3.31
3	(53)	1.50	1.70	1.80	1.35	3.00	3.35	3.83	0.55
5	(55)	3.48	5.49	3.48	5.43	6.57	5.23	4.46	1.61
7	(57)	1.35	3.06	2.95	12.74	16.68	14.13	14.47	1.58
9	(59)	11.82	15.65	9.27	1.36	1.66	3.90	3.25	14.63
11	(61)	6.89	6.88	6.51	23.73	21.09	12.83	12.14	4.16
13	(63)	1.66	3.74	1.63	1.58	2.41	3.04	6.28	2.28
14	(63)	7.42	14.84	13.41	3.84	7.08	10.32	11.78	17.77
15	(63)	2.99	5.18	5.45	6.56	7.22	10.37	10.04	14.66
17	(65)	1.66	1.44	2.11	4.52	3.63	5.03	2.71	1.52
18	(65)	1.38	1.48	0.32	5.89	4.11	3.38	2.36	0.57
19	(65)	0.94	0.85	1.33	1.54	1.49	1.35	1.06	0.48
21	(10)	0.48	0.35	0.62	1.37	1.18	1.28	1.18	0.21
23	(12)	1.68	0.53	0.60	11.40	8.42	7.36	5.90	1.61
25	(11)	3.99	2.38	2.16	1.40	1.23	1.72	1.67	0.50
27	(85)	3.08	3.63	2.43	2.77	2.28	1.90	1.67	1.27
29	(87)	3.70	3.58	2.63	0.47	0.46	0.60	0.61	0.45
30	(87)	1.52	1.64	0.12	1.57	1.18	1.05	1.10	0.16
31	(87)	0.93	0.87	0.60	1.47	0.93	0.72	1.28	0.35
33	(89)	5.53	3.77	4.35	2.27	2.12	3.00	2.94	10.07
35	(91)	3.45	1.53	2.60	1.24	1.10	1.40	1.59	1.63
37	(93)	1.44	1.77	1.53	0.64	0.13	2.23	0.39	0.67
39	(95)	3.17	2.89	3.39	0.12	0.05	0.51	0.17	3.22
43	(97)	4.48	0.53	0.86	0.29	0.42	0.28	0.22	2.23
45	(99)	8.85	6.85	10.31	0.13	0.20	0.35	0.29	6.53
47	(101)	3.32	3.51	4.83	0.20	0.18	0.14	0.08	1.28
49	(105)	6.60	5.98	5.93	1.37	2.05	2.10	3.83	6.68
51	(2)	1.37	0.90	0.51	0.08	0.05	0.33	0.11	0.31
53	N	3.40	3.13	1.21	0.17	0.15	0.46	0.16	1.06
55	W	2.11	1.79	1.83	1.59	1.22	0.63	0.73	4.19
57	E	0.90	0.59	0.61	0.10	0.13	0.31	0.29	4.03
59	S	2.34	1.44	1.55	0.09	0.20	0.23	0.08	1.15



Signature... *[signature]* ....Page 78 of 103

Table 3 (continued). Carboxylic acids

- The methyl ester of hexadecanoic acid (C_{16}) is associated with early stage decomposition.
- Long chain C_{16} fatty acids were not found in the samples, however, seven shorter chain free fatty acids in the range C_2 - C_9, acetic (C_2), propanoic (C_3), butanoic (C_4), hexanoic (C_6), heptanoic (C_7), octanoic (C_8) and nonanoic (C_9) acids were detected in the samples. In addition the aromatic compound benzoic acid was also present.
- There is a sample location difference in the distribution of the C_2-C_9 acids which is related to acid chain length. The longer C_6-C_9 (hexanoic, heptanoic, octanoic and nonanoic) acids predominate at sample locations 7, 11, 14, 15 and 23, whereas the shorter C_2-C_4 (acetic, propanoic and butanoic) acids predominate for samples 9, 14, 33, 45 and 49. Acetic and propanoic acids dominate the Northern boundary sample (53).
- The aromatic benzoic acid has abundance maxima for samples 9, 14, 15, 33, 39 – 49 and for the Western (55) and Eastern (57) boundary samples.

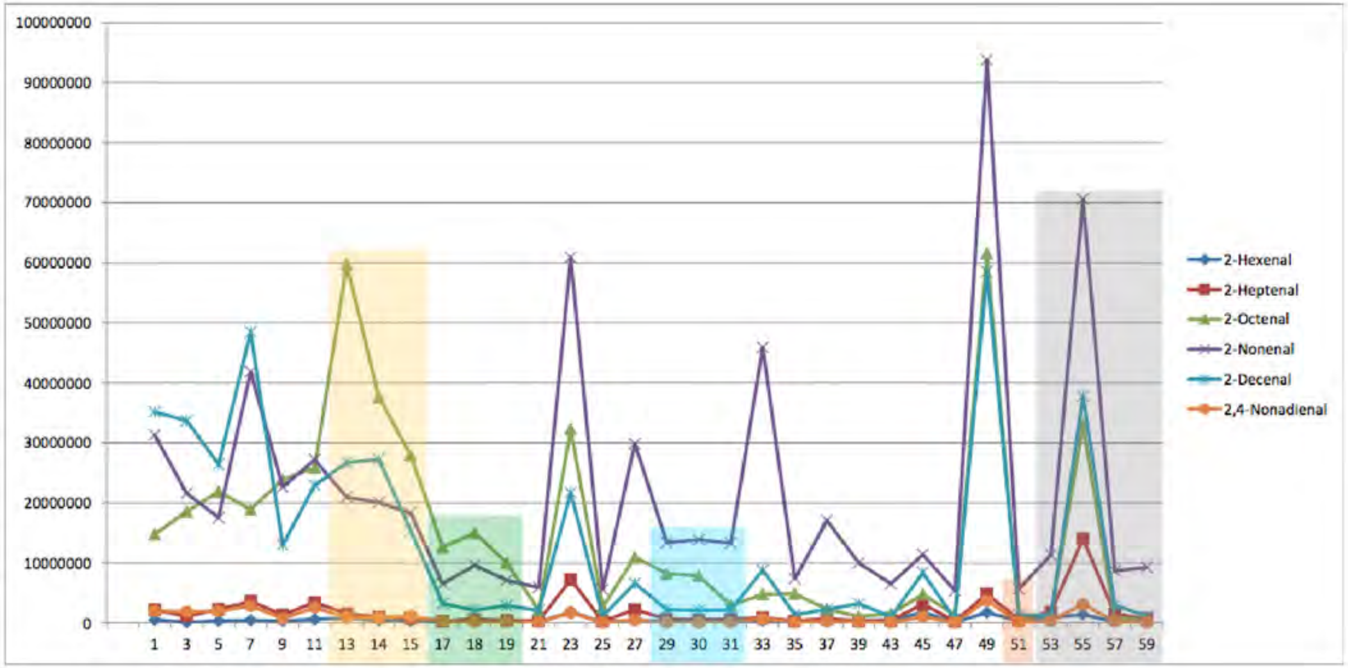
Signature... Lorna Dawson ....Page 79 of 103

Table 3 (continued). Unsaturated aldehydes (abundance per g of sample)

Sample Number	Content Number	2-Hexenal	2-Heptenal	2-Octenal	2-Nonenal	2-Decenal	2,4-Nonadienal
1	(51)	524,962	2,189,826	14,755,975	31,302,445	35,133,365	1,991,880
3	(53)	123,288	1,146,607	18,541,108	21,605,178	33,683,089	1,859,656
5	(55)	349,007	2,262,592	21,879,631	17,511,436	26,395,186	1,939,782
7	(57)	455,187	3,585,456	18,895,448	41,854,316	48,452,930	2,847,919
9	(59)	323,311	1,361,161	23,876,301	22,634,910	12,991,901	759,407
11	(61)	603,520	3,391,797	25,866,008	27,212,070	22,919,132	2,560,125
13	(63)	792,967	1,562,802	59,699,903	20,942,872	26,704,236	923,994
14	(63)	446,313	983,995	37,655,149	20,072,808	27,246,178	857,356
15	(63)	357,999	834,384	27,927,206	18,289,683	15,411,939	1,137,571
17	(65)	195,170	295,179	12,619,443	6,518,301	3,201,033	220,218
18	(65)	609,511	588,609	14,990,214	9,618,882	2,115,373	187,525
19	(65)	242,295	392,945	10,001,785	7,094,764	2,910,982	190,676
21	(10)	158,162	364,201	2,171,879	5,906,652	2,043,875	149,184
23	(12)	1,818,458	7,215,438	32,275,774	60,855,601	21,665,472	1,695,202
25	(11)	131,197	258,796	2,663,495	5,543,910	1,127,203	85,518
27	(85)	436,691	2,237,696	10,940,523	29,850,341	6,571,054	518,046
29	(87)	316,621	626,685	8,234,087	13,385,495	2,232,027	65,445
30	(87)	285,071	531,903	7,852,657	13,843,806	2,101,881	69,841
31	(87)	217,002	613,871	2,921,877	13,302,384	2,175,694	106,464
33	(89)	362,565	853,448	4,770,023	45,884,916	8,788,940	696,674
35	(91)	175,376	321,318	4,873,376	7,366,702	1,356,236	130,875
37	(93)	271,955	691,044	2,258,398	17,054,828	2,245,837	286,381
39	(95)	412,259	315,721	1,097,893	10,007,920	3,214,935	129,142
43	(97)	427,059	393,303	1,504,223	6,513,523	1,047,344	82,089
45	(99)	1,750,075	3,149,017	4,790,909	11,406,565	8,376,028	1,042,941
47	(101)	142,229	271,849	1,301,780	5,357,205	598,979	79,165
49	(105)	1,737,670	4,840,230	61,520,916	93,791,309	58,512,788	3,732,470
51	(2)	327,256	514,394	940,867	5,645,595	1,406,962	111,404
53	N	888,294	1,828,254	1,231,033	11,340,654	1,293,901	333,613
55	W	1,408,249	14,025,693	33,035,738	70,603,367	37,758,743	3,093,335
57	E	174,311	1,521,281	696,346	8,678,295	2,950,879	287,798
59	S	173,741	646,113	530,445	9,268,297	1,118,240	83,971

Signature... Lorna Dawson ....

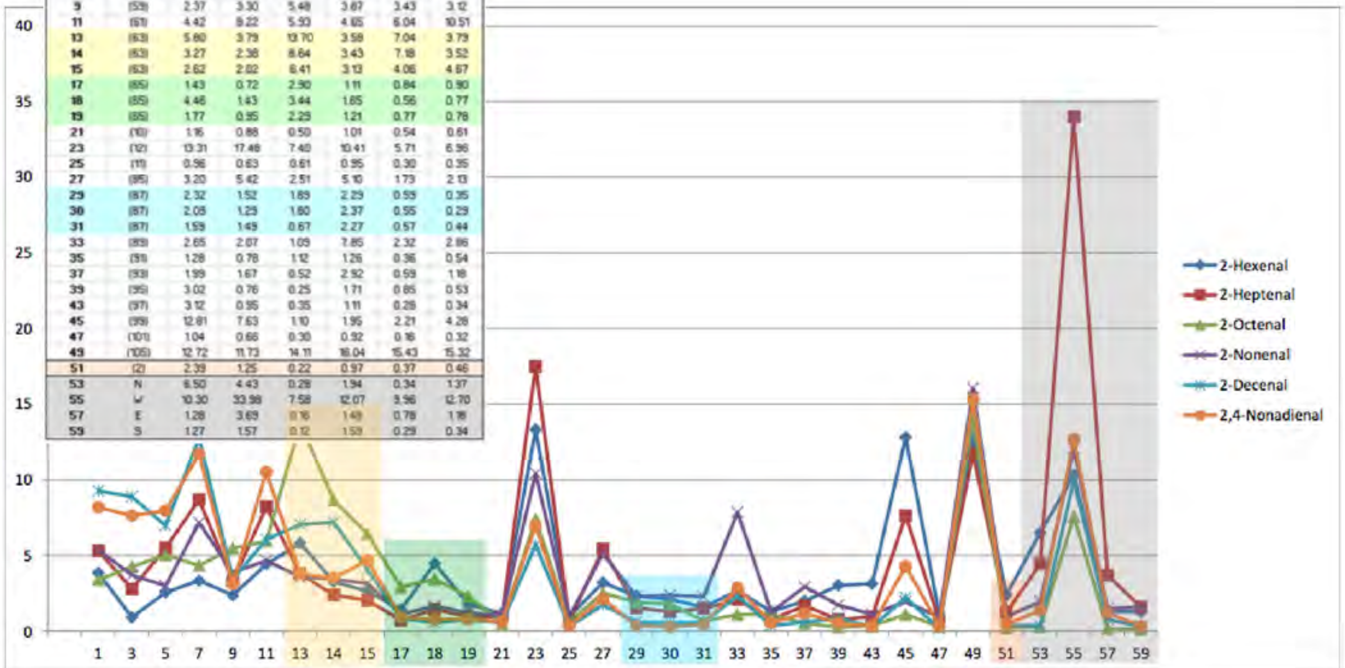
Table 3 (continued). Unsaturated aldehydes (abundance per g of sample)



Signature... ....Page 81 of 103

Table 3 (continued). Unsaturated aldehydes (abundance per sample as a percentage of the total abundance for samples 1 – 49)

Sample Number	Context Number	2-Hexenal	2-Heptenal	2-Octenal	2-Nonenal	2-Decenal	2,4-Nonadienal
1	(51)	3.84	5.30	3.39	5.35	9.26	8.17
3	(53)	0.90	2.76	4.25	3.63	8.88	7.63
5	(55)	2.55	5.49	5.02	2.99	6.96	7.96
7	(57)	3.33	8.69	4.33	7.16	12.78	11.69
9	(59)	2.37	3.30	5.48	3.67	3.43	3.12
11	(61)	4.42	8.22	5.93	4.65	6.04	10.51
13	(63)	5.80	3.79	13.70	3.58	7.04	3.79
14	(63)	3.27	2.38	8.64	3.43	7.18	3.52
15	(63)	2.62	2.02	6.41	3.13	4.06	4.67
17	(65)	1.43	0.72	2.90	1.11	0.84	0.90
18	(65)	4.46	1.43	3.44	1.65	0.56	0.77
19	(65)	1.77	0.95	2.29	1.21	0.77	0.78
21	(10)	1.16	0.88	0.50	1.01	0.54	0.61
23	(12)	13.31	17.48	7.40	10.41	5.71	6.96
25	(11)	0.96	0.63	0.61	0.95	0.30	0.35
27	(85)	3.20	5.42	2.51	5.10	1.73	2.13
29	(87)	2.32	1.52	1.89	2.29	0.59	0.35
30	(87)	2.08	1.25	1.60	2.37	0.55	0.29
31	(87)	1.59	1.49	0.67	2.27	0.57	0.44
33	(89)	2.65	2.07	1.09	7.85	2.32	2.86
35	(91)	1.28	0.78	1.12	1.26	0.36	0.54
37	(93)	1.99	1.67	0.52	2.92	0.59	1.18
39	(95)	3.02	0.76	0.25	1.71	0.85	0.53
43	(97)	3.12	0.95	0.35	1.11	0.28	0.34
45	(99)	12.81	7.63	1.10	1.95	2.21	4.28
47	(101)	1.04	0.66	0.30	0.92	0.16	0.32
49	(105)	12.72	11.73	14.11	16.04	15.43	15.32
51	(2)	2.39	1.25	0.22	0.97	0.37	0.46
53	N	6.50	4.43	0.28	1.94	0.34	1.37
55	W	10.30	33.98	7.58	12.07	9.96	12.70
57	E	1.28	3.69	0.16	1.49	0.78	1.18
59	S	1.27	1.57	0.12	1.59	0.29	0.34



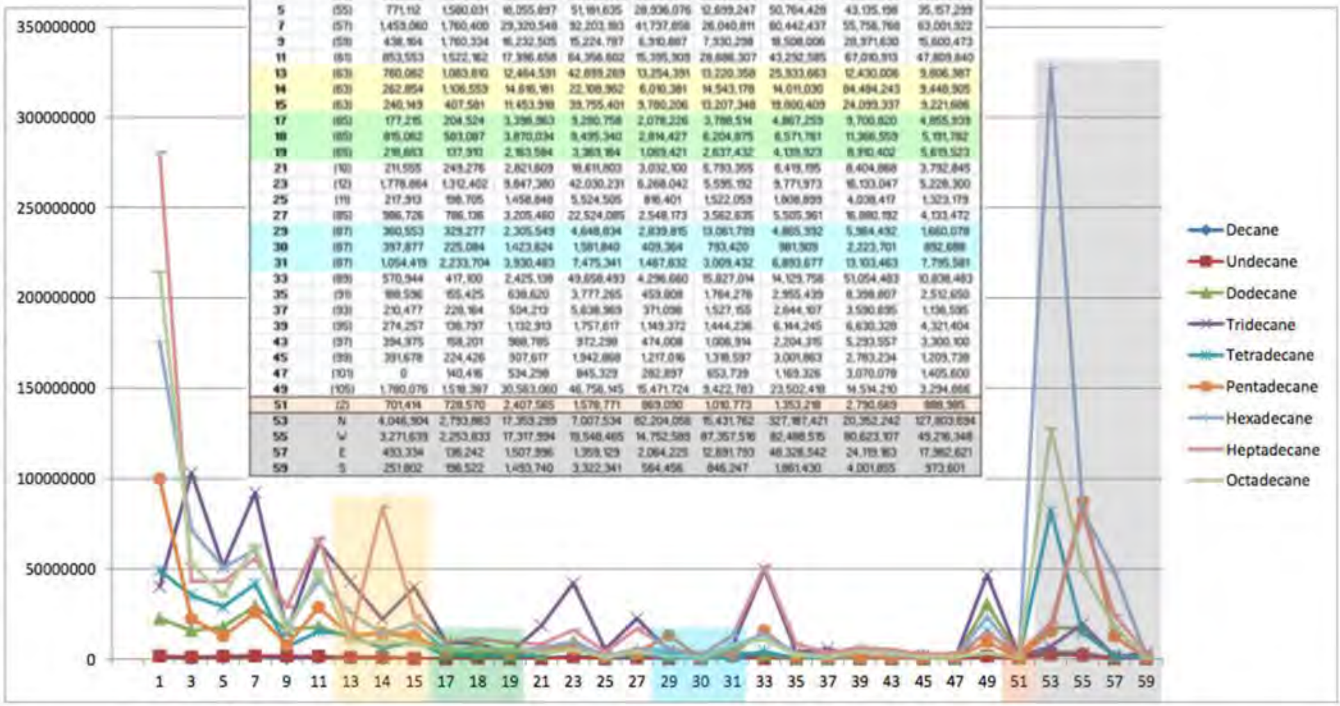
Signature... ....Page 82 of 103

Table 3 (continued). Unsaturated aldehydes

- 2-Alkenals in the range C_6 –C_{10} were detected in the samples, consisting of 2-hexenal (C_6), 2-heptenal (C_7), 2-octenal (C_8), 2-nonenal (C_9) and 2-decenal (C_{10}). In addition, 2,4-nonadienal (C_9) was also present.
- The C_8-C_{10} unsaturated aldehydes 2-octenal, 2-nonenal and 2-decenal were most abundant, followed by the C_6 and C_7 compounds 2-hexenal and 2-heptenal and the C_9 2,4-nonadienal.
- Abundance maxima were observed for samples 1-15, 23, 27, 33, 49, and for the Western boundary sample (55). This distribution profile is very similar to that seen for the saturated C_8-C_{10} *n*-aldehydes octanal, nonanal and decanal, providing further evidence for a common origin for both classes of compound.

Table 3 (continued). Alkanes (abundance per g of sample)

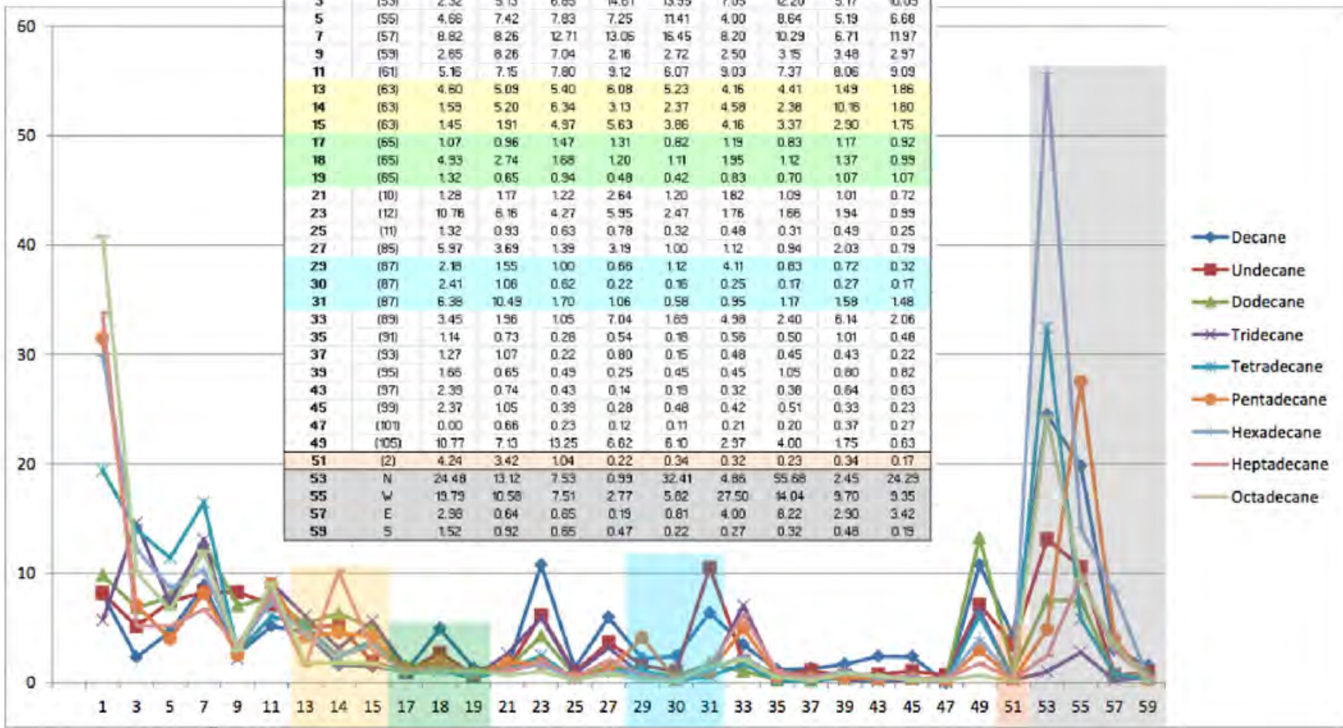
Sample Number	Context Number	Decane	Undecane	Dodecane	Tridecane	Tetradecane	Pentadecane	Hexadecane	Heptadecane	Octadecane
1	(51)	1,336,268	1,745,987	22,625,379	40,137,565	49,174,757	100,007,654	175,559,678	280,640,026	214,469,965
3	(53)	382,922	1,091,996	15,789,842	103,089,458	35,383,818	22,359,324	71,679,916	42,960,783	53,096,919
5	(55)	771,112	1,580,031	18,055,897	51,181,635	28,936,076	12,699,247	50,764,429	43,135,198	35,157,259
7	(57)	1,459,060	1,760,400	29,320,548	92,203,183	41,737,658	26,040,811	60,442,437	55,758,768	63,001,922
9	(59)	438,164	1,760,334	16,232,505	15,224,797	6,310,887	7,330,298	18,508,006	28,371,630	15,600,473
11	(61)	853,553	1,522,182	17,396,658	64,356,602	15,395,309	28,686,307	43,252,585	67,010,913	47,809,840
13	(63)	760,062	1,083,810	12,464,531	42,899,269	13,254,391	13,220,358	25,333,663	12,430,006	9,806,387
14	(63)	262,854	1,106,553	14,616,181	22,108,962	6,010,381	14,543,178	14,011,030	84,484,243	9,448,905
15	(63)	240,149	407,581	11,453,918	39,755,401	9,780,206	13,207,348	19,000,409	24,099,337	9,221,686
17	(65)	177,215	204,524	3,396,963	9,290,758	2,078,226	3,788,514	4,867,259	9,700,820	4,855,939
18	(65)	815,062	503,087	3,870,034	9,495,340	2,814,427	6,204,875	6,571,761	11,366,559	5,191,782
19	(65)	218,663	137,910	2,163,584	3,363,164	1,069,421	2,637,432	4,139,923	8,910,402	5,619,523
21	(10)	211,555	249,276	2,821,609	18,611,803	3,032,100	5,793,355	6,419,195	8,404,868	3,792,845
23	(12)	1,778,864	1,312,402	9,847,380	42,030,231	6,268,042	5,595,192	9,771,973	16,133,047	5,228,300
25	(11)	217,913	198,705	1,458,848	5,524,505	816,401	1,522,059	1,808,899	4,038,417	1,323,179
27	(85)	986,726	786,136	3,205,460	22,524,085	2,548,173	3,562,635	5,505,961	16,880,192	4,133,472
29	(87)	360,553	329,277	2,305,549	4,648,834	2,839,815	13,061,789	4,865,392	5,984,432	1,660,078
30	(87)	397,877	225,084	1,423,624	1,581,840	409,364	793,420	981,909	2,223,701	892,688
31	(87)	1,054,419	2,233,704	3,930,483	7,475,341	1,467,832	3,009,432	6,893,677	13,103,463	7,795,581
33	(89)	570,944	417,100	2,425,139	49,658,493	4,296,660	15,827,014	14,129,758	51,054,483	10,808,483
35	(91)	188,536	155,425	638,620	3,777,265	459,808	1,764,276	2,955,439	8,398,807	2,512,650
37	(93)	210,477	228,164	504,213	5,638,969	371,098	1,527,155	2,644,107	3,590,695	1,136,595
39	(95)	274,257	138,737	1,132,913	1,757,617	1,149,372	1,444,236	6,144,245	6,630,328	4,321,404
43	(97)	394,975	158,201	988,785	972,298	474,008	1,008,914	2,204,315	5,293,557	3,300,100
45	(99)	391,678	224,426	307,617	1,942,868	1,217,016	1,318,597	3,001,863	2,783,234	1,209,739
47	(101)	0	140,416	534,298	845,329	282,897	653,739	1,169,326	3,070,078	1,405,600
49	(105)	1,780,076	1,518,387	30,583,060	46,758,145	15,471,724	9,422,783	23,502,418	14,514,210	3,294,666
51	(2)	701,414	728,570	2,407,565	1,578,771	869,090	1,010,773	1,353,218	2,790,669	888,985
53	N	4,046,904	2,793,863	17,353,299	7,007,534	82,204,058	15,431,762	327,187,421	20,352,242	127,803,694
55	W	3,271,639	2,253,833	17,317,994	19,548,465	14,752,589	87,357,516	82,488,515	80,623,107	49,276,348
57	E	493,334	136,242	1,507,996	1,359,129	2,064,225	12,891,793	48,328,542	24,119,163	17,362,621
59	S	251,802	198,522	1,493,740	3,322,341	584,456	846,247	1,861,430	4,001,855	373,601



Signature... ....Page 84 of 103

Table 3 (continued). Alkanes (abundance per sample as a percentage of the total abundance for samples 1 – 49)

Sample Number	Context Number	Decane	Undecane	Dodecane	Tridecane	Tetradecane	Pentadecane	Hexadecane	Heptadecane	Octadecane
1	(51)	8.08	8.20	9.81	5.69	19.39	31.48	29.88	33.75	40.77
3	(53)	2.32	5.13	6.85	14.61	13.95	7.05	12.20	5.17	10.09
5	(55)	4.66	7.42	7.83	7.25	11.41	4.00	8.64	5.19	6.68
7	(57)	8.82	8.26	12.71	13.06	16.45	8.20	10.29	6.71	11.97
9	(59)	2.65	8.26	7.04	2.16	2.72	2.50	3.15	3.48	2.97
11	(61)	5.16	7.15	7.80	9.12	6.07	9.03	7.37	8.06	9.09
13	(63)	4.60	5.09	5.40	6.08	5.23	4.16	4.41	1.49	1.86
14	(63)	1.59	5.20	6.34	3.13	2.37	4.58	2.38	10.16	1.80
15	(63)	1.45	1.91	4.97	5.63	3.86	4.16	3.37	2.90	1.75
17	(65)	1.07	0.96	1.47	1.31	0.82	1.19	0.83	1.17	0.92
18	(65)	4.93	2.74	1.68	1.20	1.11	1.95	1.12	1.37	0.99
19	(65)	1.32	0.65	0.94	0.48	0.42	0.83	0.70	1.07	1.07
21	(10)	1.28	1.17	1.22	2.64	1.20	1.82	1.09	1.01	0.72
23	(12)	10.76	6.16	4.27	5.95	2.47	1.76	1.66	1.94	0.99
25	(11)	1.32	0.93	0.63	0.78	0.32	0.48	0.31	0.49	0.25
27	(85)	5.97	3.69	1.39	3.19	1.00	1.12	0.94	2.03	0.79
29	(87)	2.18	1.55	1.00	0.66	1.12	4.11	0.83	0.72	0.32
30	(87)	2.41	1.06	0.62	0.22	0.16	0.25	0.17	0.27	0.17
31	(87)	6.38	10.49	1.70	1.06	0.58	0.95	1.17	1.58	1.48
33	(89)	3.45	1.96	1.05	7.04	1.69	4.98	2.40	6.14	2.06
35	(91)	1.14	0.73	0.28	0.54	0.18	0.56	0.50	1.01	0.48
37	(93)	1.27	1.07	0.22	0.80	0.15	0.48	0.45	0.43	0.22
39	(95)	1.66	0.65	0.49	0.25	0.45	0.45	1.05	0.80	0.82
43	(97)	2.39	0.74	0.43	0.14	0.19	0.32	0.38	0.64	0.63
45	(99)	2.37	1.05	0.39	0.28	0.48	0.42	0.51	0.33	0.23
47	(101)	0.00	0.66	0.23	0.12	0.11	0.21	0.20	0.37	0.27
49	(105)	10.77	7.13	13.25	6.62	6.10	2.97	4.00	1.75	0.63
51	(2)	4.24	3.42	1.04	0.22	0.34	0.32	0.23	0.34	0.17
53	N	24.48	13.12	7.53	0.99	32.41	4.86	55.68	2.45	24.29
55	W	19.79	10.58	7.51	2.77	5.82	27.50	14.04	9.70	9.35
57	E	2.98	0.64	0.65	0.19	0.81	4.00	8.22	2.90	3.42
59	S	1.52	0.92	0.65	0.47	0.22	0.27	0.32	0.48	0.19



Signature... ....Page 85 of 103

Table 3 (continued). Alkanes

- Straight chain (*n*-) alkanes in the range C_5-C_{11} are associated with mammalian decomposition and the longer homologues are particularly associated with human decomposition, for which the presence of undecane (C_{11}) is considered to be a marker.
- The C_{10}-C_{18} alkane homologues decane (C_{10}), Undecane (C_{11}), dodecane (C_{10}), tridecane (C_{13}), tetradecane (C_{14}), pentadecane (C_{15}), hexadecane (C_{16}) heptadecane (C_{17}) and octadecane (C_{18}) were found in the samples.
- For most alkane homologues there is a broad abundance maxima profile over samples 1 – 15 and also at samples 23, 27, 31, 33 and 49, and at the Northerly (53) and to a lesser extent the Westerly (55) boundary samples.
- Maximum alkane abundances were seen for the longest C_{15}-C_{18} homologues, pentadecane, hexadecane, heptadecane and octadecane at the most easterly cell (sample 1), and for tetradecane, hexadecane and octadecane at the Northerly (53) boundary sample.
- Undecane (C11) was generally of low abundance in all samples, but the abundance maxima for this compound were for samples 1-14, 23, 27, 31, 49, and for the boundary samples 53 and 55.

Signature... Lorna Dawson

Appendix 5

Solid organic compound analysis

***Derivatisation of compounds of interest prior to analysis by gas chromatography*:**

The use of **BSTFA** reagent to convert any alcohol species present in the soil 'alcohol' fractions to **trimethylsilyl (TMS) ethers** not only improves gas-chromatographic separations, but with **GCMS** allows direct identification of peaks appearing on the gas chromatogram, since the individual **TMS** compounds have distinct characteristic mass spectra. Similarly, methylation of the carboxyl groups of organic acids improves improves gas-chromatographic separations; for hydroxyacids, such as the faecal bile acids and 10-hydroxystearic acid, to get good separations and distinct mass spectra, it is necessary to both methylate the carboxyl group and silylate the hydroxyl groups on the compounds.

***Gas chromatography (GC)*:** This is a method of separating and quantifying individual components (compounds) from complex mixtures, based on differences in relative affinities for a stationary phase (usually an immobilised liquid) and remaining in a vapour phase. The sample is introduced to a column (long tube) as a vapour, which is swept along the column by flow of an inert **carrier gas** (commonly nitrogen, helium or hydrogen). In the past, most gas chromatography was carried out using *packed columns* in which the stationary phase was supported by inert particles held throughout the length of the column. Most present-day applications involve the use of *capillary columns*, in which the stationary phase coats the inside of long, narrow silica, glass or metal tubing; capillary columns have much higher resolutions. As the sample vapour passes along the column, different components travel at differing rates, leading to separation of the components into individual peaks leaving the distal end of the column. The speed of passage and degree of separation is affected by the amount of stationary phase, carrier gas flow rate and column temperature. The instrument containing the column, the **gas chromatograph**, consists primarily of a temperature-programmable oven which encloses the column. Unless the sample is a gaseous mixture, samples to be analysed are usually dissolved in a volatile solvent, and introduced by means of a syringe, either directly onto the column (e.g. *cold on-column injection*), or an injection system, heated to vaporise the sample; the sample vapours are swept on to the column by the carrier gas. The separated sample component peaks reaching the lower end of the column are sensed by a *detector*, which gives an electrical response dependent on the size of the component peak. There are a number of different types of detector, dependent upon the components being analysed. For routine analysis of organic compounds the *flame ionisation detector* is most widely used. Some modern gas chromatography columns have been designed to allow compounds of relatively low volatility to be analysed, by running at high temperatures. The plant wax compounds and sterols/stanols described in the present report come under this category.

Gas chromatography-mass spectrometry (GCMS): This is essentially conventional gas chromatography fitted with a mass-selective detector, primarily for resolution of organic analytes. The separated compound molecules eluting from the chromatography column are transferred to a vacuum chamber, where they are ionised and separated and detected according to ion mass. In the most widely used configuration (as used in the work described in this report), the analyte molecules are ionised by bombardment with an electron beam (*electron ionisation*), which breaks up the molecules to produce a number of fragment ions. By using a fixed standard electron energy (conventionally 70eV), the relative percentages of the different fragment ions result in a reproducible *mass spectrum* which, being characteristic for different individual compounds, enables the compounds to be directly identified. Since the number of ions produced for a particular compound is dependent on the amounts of compound eluting from the GC column, quantitative analysis can be carried out. Counting all of the ions produced (*total ion count*, TIC) results in a gas chromatogram which is very similar to that obtained from a conventional gas chromatograph fitted with a flame ionisation detector.

Interpretation of gas chromatograms and quantification: In conventional gas chromatography, compound peaks can be identified from the *retention time*, which is the time after injecting the sample that the summit of the peak occurs; standard mixtures containing compounds of interest also need to be run under identical conditions (temperature, gas flow rate etc.) of the gas chromatograph. Peak sizes are usually determined in terms of peak areas, determined with specialist software built into a computing integrator or computer attached to the gas chromatograph. The accurate assessment of peak area is very much dependent on the correct positioning of baselines executed by the software; this is particularly important in situations where peaks may not be fully resolved.

The *n*-alkanes, fatty alcohols, sterols and stanols in the samples analysed in this report could be quantified by adding a known amount of relevant *internal standard* compound to the sample prior to extraction, purification and analysis. Ideally, a suitable internal standard compound should not be present in the samples, but have the same physical and chemical properties as the compounds being quantified. It has been shown that the concentrations of the chosen internal standards for *n*-alkanes and for fatty alcohols can be considered as having negligible concentrations in plant and soil samples. The internal standard used to quantify *n*-alkanes was tetratriacontane (C34).The fatty alcohol internal standard was1-heptacosanol (C27-ol), the fatty acid standard was hentriacontanoic acid (C31) and 5β-cholan-24-ol was added as the internal standard for the sterols and stanols.

A mixture of standards of some of the main alcohols and sterols expected to be found in the samples were run on the GC-MS to corroborate retention times and identification.

ORGANIC MARKERS RELEVANT TO THIS REPORT

Plant wax compounds: Lipid (hydrophobic) compounds found in the surface wax of plants. These can be complex mixtures. The plant wax compounds mentioned in this report are listed as follows:
***n*-Alkanes**: straight-chain, C_{21}-C_{37}, with odd-chain compounds predominating

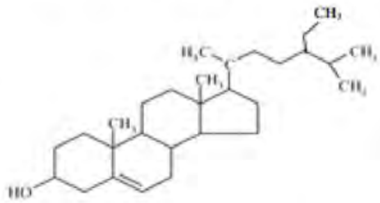
Primary long-chain fatty alcohols: straight-chain, C_{20}-ol - C_{34}-ol, predominantly even-chain

Sterols and stanols:

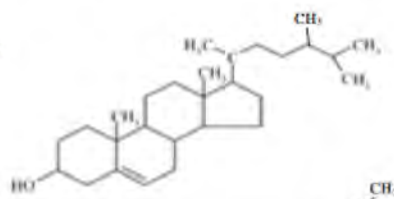
These, if present, occur in the 'alcohol' fraction eluted from silica-gel columns. Sterols are unsaturated (i.e. containing one or more double bonds) steroidal alcohols; stanols are saturated steroidal alcohols.

Sterols:

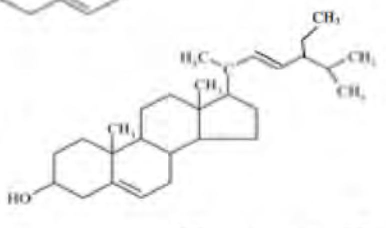
β-Sitosterol (24-ethyl cholest-5-en-3β-ol):
main sterol found in plants



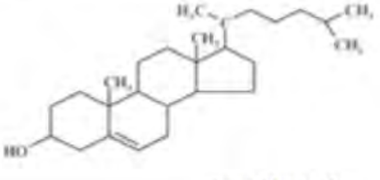
Campesterol (24-methyl cholest-5-en-3β-ol):
common plant sterol



Stigmasterol (24-ethyl 5,22-dien-cholestan-3β-ol)
common plant sterol



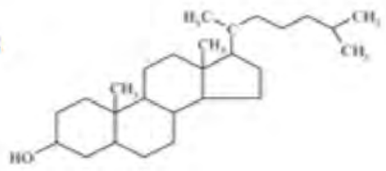
Cholesterol (cholest-5-en-3β-ol):
main sterol found in animals



Signature... ....Page 89 of 103

Stanols:

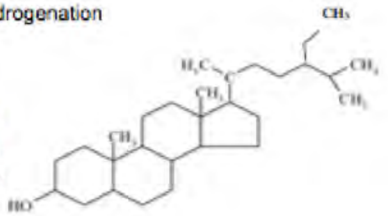
Coprostanol (5β-cholestan-3β-ol): hydrogenation product of cholesterol occurring in mammalian faeces; main stanol in human and pig faeces



Epicoprostanol (5β-cholestan-3α-ol): isomer produced from coprostanol by microbes under anaerobic conditions (e.g. septic tank)

Cholestanol (5α-cholestan-3β-ol): another isomer produced by hydrogenation of cholesterol under anaerobic conditions in the environment (not in the mammalian gut).

24-Ethylcoprostanol (24-ethyl 5β-cholestan-3-β-ol): hydrogenation product of β-Sitosterol; main stanol in herbivore faeces



24-Ethyl epicoprostanol (24-ethyl 5β-cholestan-3α-ol): isomer produced from 24-ethylcoprostanol by microbes under anaerobic conditions (e.g. farm slurry tank); minor stanol in fresh faeces

Stigmastanol (24-ethyl 5α-cholestan-3β-ol):
another isomer produced by hydrogenation of β-sitosterol under anaerobic conditions in the environment (not in the mammalian gut:

Campestanol (24-methyl 5α-cholestan-3β-ol): hydrogenation product produced by hydrogenation of campesterol under anaerobic conditions in the environment (not in the mammalian gut).

NB: The structural diagrams of the above stanols and isomers are generic. The numbers refer to the individual carbon atoms within the steroidal structure and the Greek letters (α and β) refer to whether the side group (e.g. the 'OH' group) is in a position above or below the ring structure. The same applies to 24-ethylcoprostanol, campestanol and their isomers.

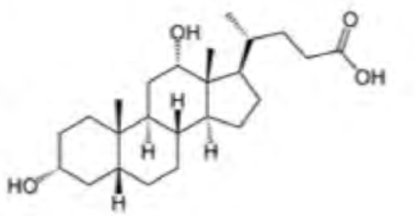
Signature... Lorna Dawson ....Page 90 of 103

Faecal bile acids:

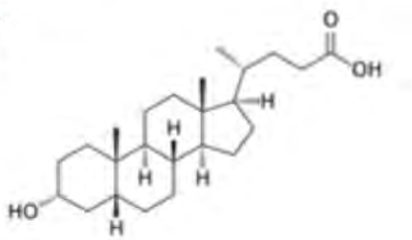
Bile acids are steroidal hydroxyl acids. The compounds of interest as markers found in faeces are secondary bile acids, which have been transformed by gut bacteria from primary bile acids (cholic acid and chenodeoxycholic acid) which had been secreted into the gut from bile.

Lithocholic acid (3α-hydroxy-5β-cholan-24-oic acid):

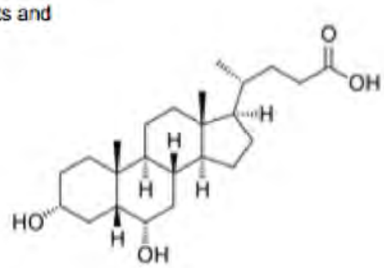
found in faeces of most mammals, including faeces from humans, pigs, ruminants and other herbivores.



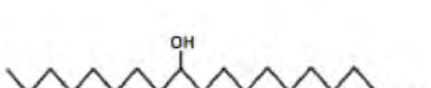
Deoxycholic acid (3α,12α-dihydroxy-5β-cholan-24-oic acid): found in faeces of humans, ruminants and other herbivores, but not in pig faeces



Hyodeoxycholic acid (3α,6α-dihydroxy-5β-cholan-24-oic acid): found in pig faeces, but not in faeces of humans, ruminants and other herbivores



10-Hydroxy stearic acid:



Produced from oleic acid by microbes under wet anaerobic conditions. It is a major constituent of adipocere, which is a white soapy substance originating from body fat and found in cadavers which had decomposed in a waterlogged environment. 10-Hydroxystearate is thus a useful body decomposition marker and has also been found in human faeces.

Summary of procedure for the analysis of soil samples for organic lipid markers

High-purity solvents are re-distilled (*n*-heptane, ethanol and ethyl acetate) before being used.

The air-dried soil samples were hand milled in an agate mortar and pestle. Duplicate sub-samples of each soil (about 100mg) were weighed with alkane, fatty alcohol, fatty acid and sterol internal standard compounds from separate solutions of known concentration (C22 and C34 *n*-alkanes, C27 alcohol, C31 acid and 5β-cholan 24ol, respectively) into screw capped tubes with PTFE cap-liners, and heated overnight in sealed screw-cap vials with 1M ethanolic KOH at 90°C.

After cooling to 50°C and the addition of water, any hydrocarbons (including *n*-alkanes) and alcohols present were extracted twice with *n*-heptane. After removing the solvent, the heptane extracts were re-dissolved in heptane prior to being transferred to a small glass solid-phase extraction column packed with about 50mg of silica-gel. The hydrocarbons were eluted from the column with *n*-heptane. The solvent was then changed to 20% ethyl acetate/ 80% *n*-heptane (v/v) in order to elute any fatty alcohols, sterols and triterpenols (crude alcohol extract). The hydrocarbon extract was dried and redissolved in dodecane prior to analysis by GC. The crude alcohol extract was derivitised with a mixture of BSTFA and pyridine before drying and redissolving in dodecane prior to analysis by GC-MS.

The residue remaining after alkane and alcohol extraction was acidified and extracted with chloroform. The extracted compounds were added to an SPE column containing aminopropyl packing. The organic acids were eluted with a mixture of diethyl ether and glacial acetic acid. After drying the acids were converted to their methyl esters, by heating with acidified methanol and then further treated with BSTFA to silylate the hydroxyl groups (as trimethylsilyl ethers on hydroxy acids). The derivatised extracts were analysed by GCMS in TIC mode.

Appendix 6

Isotope analysis

The method used was according to the James Hutton Institute - 1917 Schedule, AM002. The carbon and nitrogen concentrations (%) along with $\delta^{13}C$ and $\delta^{15}N$ natural abundance isotope ratios of the milled dried soil were determined using a Flash EA 1112 Series Elemental Analyser connected via a Conflo III to a Delta^{Plus} XP isotope ratio mass spectrometer (all Thermo, Bremen, Germany). The $\delta^{13}C_{VPDB}$ and $\delta^{15}N_{Air-N2}$ values were normalized to their respective scales using International Atomic Energy Agency reference materials USGS40 and USGS41a (both L-glutamic acid). Additionally the USGS40 was used as a reference material for both carbon and nitrogen concentrations, measured using the area output of the mass spectrometer (JHI – UKAS Accreditation Schedule 1917, Method AM002). Long term precisions for a quality control standard (dried milled topsoil) were: total carbon 3.80 ± 0.15 %, $\delta^{13}C$ -27.79 ± 0.20 ‰, total nitrogen 0.28 ± 0.02 % and $\delta^{15}N$ 4.63 ± 0.60 ‰ (mean ± sd). Data processing was performed using Isodat 2.0 (Thermo Fisher Scientific, Bremen, Germany) and exported into Excel.

Appendix 7

Glossary

Isotope- Atoms of an element with the normal number of protons and electrons, but different numbers of neutrons. The different isotopes of an element have identical chemical properties.

Mineral - A mineral is a naturally occurring solid chemical substance, formed through geological processes, which has a characteristic chemical composition, a highly ordered atomic structure, and specific physical properties consequent upon its structure and chemistry.

Organic - Pertaining to a class of chemical compound that exist in or have been derived from plants or animals.

VOC – Volatile organic compound is an organic chemical which is emitted as gas from certain solids or liquids.

Appendix 8

Statistical analysis

Multidimensional scaling analysis (MDS) plots analysed with Primer 6 software

Figure 2. MDS plot of VOC data.

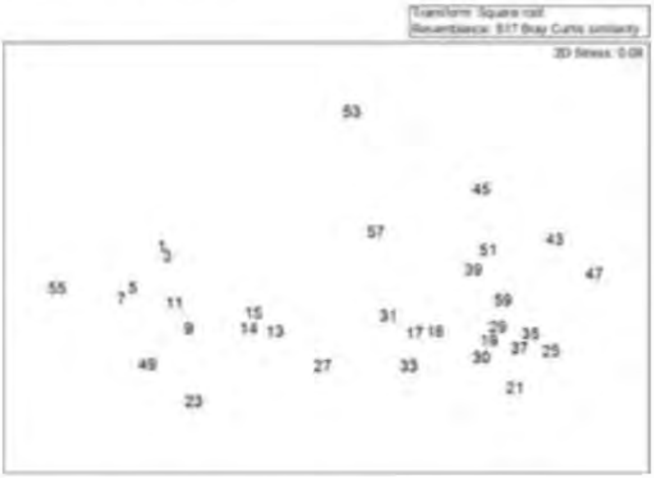


Figure 3. MDS plot of sterol and stanol data.

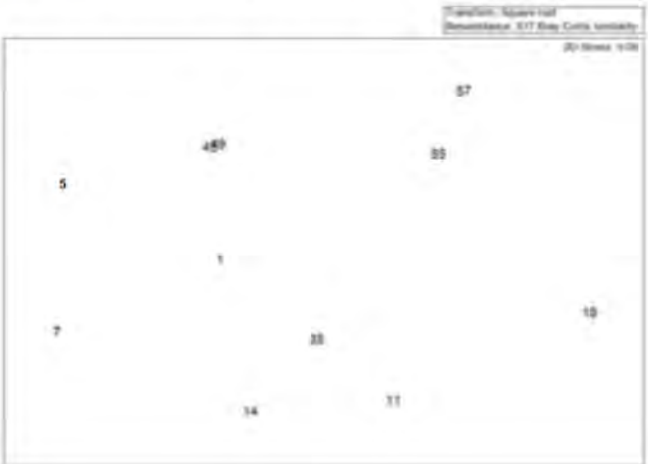


Figure 4 MDS plot of bile acid data.

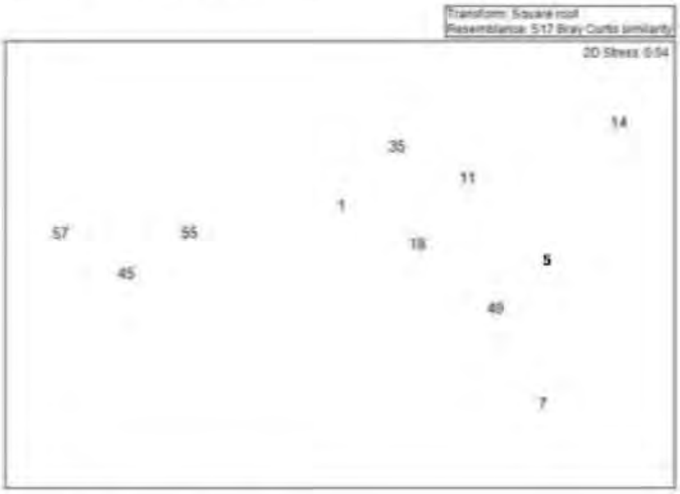
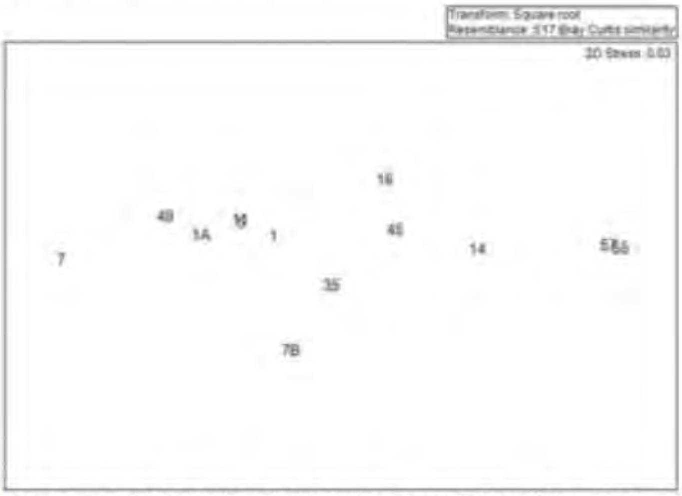


Figure 5. MDS plot of isotope data.



Note: Sample 1A is EXHIB –LL016 which we received on 4th Nov 2016.
Sample 7B is a fragment picked out from sample 7 which was thought to be bone.

Signature... *[signature]* ....Page 97 of 103

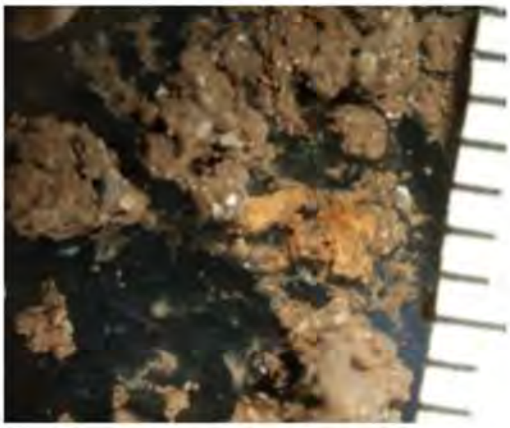
Appendix 9

Images of soil examined

Photographs of soil sample examined. (Scale = mm)

Plate 1. Sample 1

Plate 2. Sample 5



Signature... *[signature]* ....Page 98 of 103

Plate 3. Sample 7

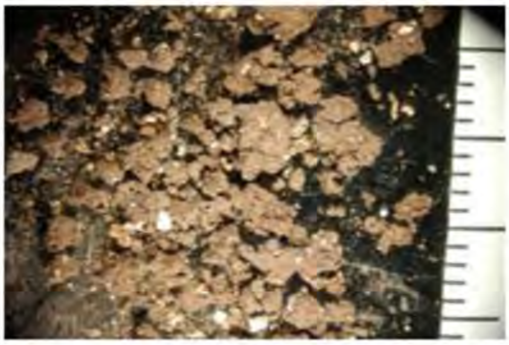


Plate 4. Sample 11

Plate 5. Sample 14

Signature... Lorna Dawson ....Page 99 of 103

Plate 6. Sample 18

Plate 7. Sample 35

Plate 8. Sample 45

Signature... ....Page 100 of 103

Plate 9. Sample 49

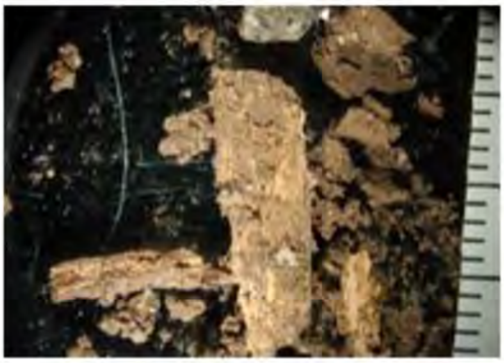
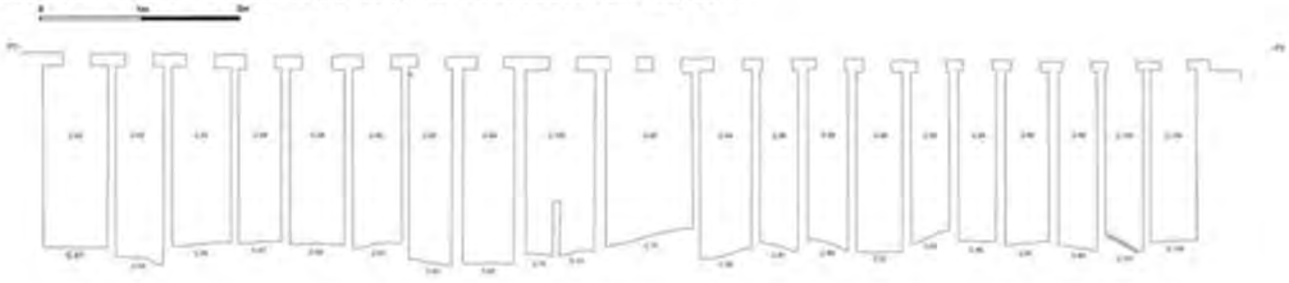


Plate 10. Sample 55

Plate 11. Sample 57

Appendix 10

Section drawing of cell locations as provide by Niamh McCULLAGH on 7 May 2017.



Signature ....Page 102 of 103

Appendix 11

Declaration

If you have any queries in relation to this report or any of the work that we have performed then please contact the laboratory.

Report provided by: Prof Lorna DAWSON, Dr Tom SHEPHERD and Dr Bob MAYES
Mrs Jasmine ROSS has quality checked this report.

Signature:

Signature:

Signature:

Address *The James Hutton Institute*
Aberdeen
AB15 8QH

Email: lorna.dawson@hutton.ac.uk

Telephone number: *01224 395328, mobile: 07815 178093*

Dated the 23rd May 2017

Signature ....Page 103 of 103

Appendix VIII: References

Bass, W. M. 1995. *Human Osteology: A Laboratory and Field Manual.* Missouri Archaeological Society, Columbia, Miss.

Haglund, W. D. & Sorg, M. H. 2002. Human Remains in Water Environments. In Haglund, W. D. & Sorg, M. H. (eds.), *Advances in Forensic Taphonomy. Method, Theory, and Archaeological Perspectives*, 201-218. CRC Press, Boca Raton.

Humphrey, L. T. & Scheuer, L. 2006. Age of Closure of the Foramen of Huschke: An Osteological Study. *International Journal of Osteoarchaeology* 16**,** 47-60.

Maresh, M. M. 1970. Measurements from Roentgenograms. In Mccammon, R. W. (ed.) *Human Growth and Development*, 157-200. C. C. Thomas, Springfield.

Mays, S. 1998. *The Archaeology of Human Bones.* Routledge, London.

McCullagh, N. 2016. Results of Phase II Site Investigations at the Reported 'Children's Burial Ground', Dublin Road Housing Estate, Tuam, Co. Galway. Unpublished Report, Report to the Mother and Baby Home Commission of Investigation, 15th December 2016.

Schaefer, M., Black, S. & Scheuer, L. 2009. *Juvenile Osteology. A Laboratory and Field Manual.* Elsevier, Amsterdam.

Utsi, E. 2015. Report tothe Independent Commission of Investigation (Mother and Baby Homes and certain related matters) on the Findings from the Geophysical Surveys of the Memorial Garden, Tuam. Unpublished Report, Report to the Mother and Baby Home Commission of Investigation, 113th November 2015.

White, T. D. & Folkens, P. A. 1991. *Human Osteology.* Academic Press, San Diego.

Addendum to Report
The Characterisation of Samples
For Niamh McCullagh and
The Mother and Baby Homes Commission of Investigation

(Criminal Procedure Rules [2015] Parts 16 and 19; Criminal Justice Act 1967, s. 9)

Report of Professor Lorna DAWSON, Dr Tom SHEPHERD and Dr Bob MAYES

Qualifications
BSc, PhD, C.Sci, F.I.Soil Sci, FRSA (LD);
BSc, PhD (TS);
BSc, MSc, PhD (BM),

Age Over 18

Occupations Soil Scientist, Volatile Organic Chemist and Organic Chemist

Address James Hutton Institute
Craigiebuckler
Aberdeen
AB15 8QH

I (Lorna DAWSON, Tom SHEPHERD and Bob MAYES) DECLARE THAT:

1. I understand that my duty is to help the court to achieve the overriding objective by giving independent assistance by way of objective, unbiased opinion on matters within my expertise, both in preparing reports and giving oral evidence. I understand that this duty overrides any obligation to the party by whom I am engaged or the person who has paid or is liable to pay me. I confirm that I have complied with and will continue to comply with that duty.

2. I confirm that I have not entered into any arrangement where the amount or payment of my fees is in any way dependent on the outcome of the case.

3. I know of no conflict of interest of any kind, other than any which I have disclosed in my report.

4. I do not consider that any interest which I have disclosed affects my suitability as an expert witness on any issues on which I have given evidence.

5. I will advise the party by whom I am instructed if, between the date of my report and the trial, there is any change in circumstances which affect my answers to points 3 and 4 above.

6. I have shown the sources of all information I have used.

7. I have exercised reasonable care and skill in order to be accurate and complete in preparing this report.

8. I have endeavoured to include in my report those matters, of which I have knowledge or of which I have been made aware, that might adversely affect the validity of my opinion. I have clearly stated any qualifications to my opinion.

9. I have not, without forming an independent view, included or excluded anything which has been suggested to me by others including my instructing lawyers.

10. I will notify those instructing me immediately and confirm in writing if for any reason my existing report requires any correction or qualification.

11. I understand that:

    (a) my report will form the evidence to be given under oath or affirmation;

    (b) the court may at any stage direct a discussion to take place between experts;

    (c) the court may direct that, following a discussion between the experts, a statement should be prepared showing those issues which are agreed and those issues which are not agreed, together with the reasons;

    (d) I may be required to attend court to be cross-examined on my report by a cross-examiner assisted by an expert.

    (e) I am likely to be the subject of public adverse criticism by the judge if the Court concludes that I have not taken reasonable care in trying to meet the standards set out above.

12. I have read Part 19 of the Criminal Procedure Rules and I have complied with its requirements.

13. I confirm that my discipline does not have a material code to adhere to.

14. I confirm that I have read guidance contained in a booklet known as *Disclosure: Experts' Evidence and Unused Material* which details my role and documents my responsibilities, in relation to revelation as an expert witness. I have followed the guidance and recognise the continuing nature of my responsibilities of disclosure. In accordance with my duties of disclosure, as documented in the guidance booklet, I confirm that:

    (a) I have complied with my duties to record, retain and reveal material in accordance with the Criminal Procedure and Investigations Act 1996, as amended;

    (b) I have compiled an Index of all material. I will ensure that the Index is updated in the event I am provided with or generate additional material;

    (c) in the event my opinion changes on any material issue, I will inform the investigating officer, as soon as reasonably practicable and give reasons.

I confirm that the contents of this report are true to the best of my knowledge and belief and that I make this report knowing that, if it is tendered in evidence, I would be liable to prosecution if I have wilfully stated anything which I know to be false or that I do not believe to be true.

Signed Lorna Dawson — Dated the 26th June 2017

Signed Tom Shepherd. — Dated the 26th June 2017

Signed R.W. Mayes — Dated the 26th June 2017

Table of Contents

1. Qualifications and Experience

Prof. Lorna DAWSON

I am employed as a principal research scientist at the James Hutton Institute, Aberdeen, Scotland, where I am Head of the Soil Forensics Section and hold the qualifications of BSc (Honours) Geography (Edinburgh University, 1979), and a PhD in Soil Science (Aberdeen University, 1984). I am a visiting Professor in Forensic Science at the Robert Gordon University. I am a Fellow of the British Society of Soil Science, a Fellow of the Royal Society of the Arts, a Chartered Scientist and hold an Expert Witness certificate in both Criminal and Civil Law (Cardiff University, 2011, 2012). I have published widely on the subject of forensic soil science; published over 80 refereed publications, books and book chapters. I am an Expert Advisor with the National Crime Agency, have worked with numerous police forces in Scotland, England, Wales, Ireland & Australia over the last 12 years and have advised on over 100 cases, written over 70 Expert Witness reports, and presented evidence in 10, in the UK and overseas. During the past 12 years I have encountered the evidence type involved in this case on several occasions.

Dr Tom SHEPHERD

I am a senior research chemist employed at the James Hutton Institute, Dundee, Scotland holding the qualifications of BSc (Honours) Chemistry (University of St Andrews, 1980) and a PhD in Synthetic Organic Chemistry (University of St Andrews, 1983). I am an expert in the use of techniques such as automated thermal desorption (ATD) and solid-phase micro-extraction (SPME), coupled with GC-MS, for entrainment and analysis of volatiles. A main element of my research is the analysis of volatile chemicals, compiling an extensive database of chromatographic characteristics from a wide range of different matrices. During the past two years I have encountered the evidence type involved in this case on several occasions.

Dr Bob MAYES

I am a Research Associate at the James Hutton Institute where I was previously head of the Ecological Sciences GC and GC-MS laboratories, and hold the qualifications PhD from Queen's University of Belfast, MSc in Animal Nutrition from the University of Aberdeen and BSc in Physiology and Biochemistry of Farm Animals from Reading University. I am an expert in the analysis of wax markers and my research interests revolve around the application of this biomarker technology to measuring dietary intake, digestibility and plant species composition in grazing herbivores and to the chemical characterisation of soil organic matter as applied in criminal investigations. I have worked with a number of police forces in Scotland, England, Wales & Ireland over the last 6 years, have written over 16 Expert Witness reports, and presented evidence in court with two of them. During the past 6 years I have encountered the evidence type involved in this case on several occasions.

2. Addendum to summary of findings

Summary from first report on sample received 4th November 2016

1.1 The sample examined was not a typical soil. It was shown from GC-MS analysis that there are markers of faeces (cholesterol, faecal stanols and faecal bile acids) in the sample.

1.2 The observed patterns of these individual markers were typical of human faeces, and not of faeces from any herbivore (e.g. sheep, cattle, horses or rabbits), pigs or dogs.

1.3 However, despite the high organic matter content of the sample, the concentrations of faecal markers were extremely low, compared with levels expected from decomposed faecal material (such as sewage sludge, septic tank sludge or manure). Thus either the faecal material had been considerably diluted by the presence of non-faecal organic matter, or the faecal markers had come from another source.

1.4 The possibility that the faecal markers found in the sample had originated from decomposing cadavers is a possibility.

1.5 The fatty acid, 10-hydroxy stearic acid, which is a recognised body decomposition marker, was found in the sample at low levels, but its origin in this case was not clear, because it is also found in human faeces. Any association of cadaver decomposition with the presence of faecal bile acids has yet to be established.

1.6 An unusual feature about the *n*-alkane/alcohol/sterol results of the sample examined was the exceptionally high levels of the plant sterols, β-sitosterol and campesterol, together with low (but detectable) concentrations of plant-wax *n*-alkanes and fatty alcohols. The observed *n*-alkane and long-chain fatty alcohol patterns were typical of those found in grasses and other higher plants, but their low concentrations relative to the plant sterol levels in the sample suggest that decomposed plant material was unlikely to be the source of these compounds in this sample.

1.7 There is the possibility that it was infant matter that was in the sample (including infant faecal matter) and that the high levels of plant sterols we detected in the sample could be as a result of infants being fed with formula milk containing vegetable oils. (Nearly all formula milks contain vegetable oils). The relative levels of plant sterols, *n*-alkanes and fatty alcohols in vegetable oils are similar to those found in the current analysed sample. Furthermore, although the patterns of *n*-alkanes and fatty alcohols can vary according to the type of vegetable oil, the patterns found in the sample examined were compatible with certain individual oils, or mixtures of oils.

1.8 The concentration patterns of stanols and sterols and hydrocarbons found in the sample are not compatible with that of sewage from human adults or from individuals eating solid food.

1.9 The alcohol/sterol fraction and hydrocarbon fraction profiles suggest that the sample examined is not material originating from a sewage treatment plant, septic tank or cesspit. It is unlikely that the specific location of the questioned case sample was a receptacle for sewage.

1.10 The sample does contain indicators which suggest that human faeces are present. However, the markers present are not compatible with that of sewage from human adults or children eating solid food. It has not originated wholly from a sewage treatment plant or wholly from adult faeces.

Summary of findings from second report on samples received on 15th February 2017

- 2.1 It can be confirmed from our examination that there is evidence that the site *had* previously been used as a sewage facility. Cholesterol, faecal stanols (coprostanol, epicoprostanol, 24-ethyl coprostanol and 24-ethyl epicoprostanol) and faecal bile acids (biomarkers found in human sewage) were detected in all samples analysed for solid organic compounds. However, during decomposition of animal (including human) bodies large quantities of cholesterol are released; coprostanol and epicoprostanol have also been found in association with body decomposition. Whilst these biomarkers are found both in sewage and in decomposing bodies, the relative concentration patterns would be expected to differ greatly between faecal (sewage) and body decomposition origins – in faeces and sewage, cholesterol concentrations are much lower than those of coprostanol + epicoprostanol, whereas cholesterol concentrations in body decomposition material would be expected to be considerably higher than these stanol concentrations. The high stanol: cholesterol ratio (Figure 2) found in sample 11 suggests that for this sample, the solid biomarkers had originated from predominantly sewage; the lower ratios observed in the other samples from the chambers suggest mixed origins from sewage and from decomposed bodies. Whilst the presence of faecal bile acids suggests that sewage had at some time in the past been present in all of the chambers providing the analysed samples, the possibility that faecal bile acids can be released during body decomposition cannot be categorically ruled out;

currently, there does not appear to be any published evidence that faecal bile acids are produced during the process of human or animal body decomposition.

Other points:

- o Coprostanol and epicoprostanol are produced in the guts of most mammals by microbial hydrogenation of cholesterol (endogenous and from dietary animal products). 24-Ethyl coprostanol and 24-ethyl epicoprostanol are produced in the gut from β-sitosterol (from dietary plant products).
- o In human sewage coprostanol+epicoprostanol concentrations are normally one to three times the concentrations of 24-ethyl coprostanol+24-ethyl epicoprostanol. If much of the coprostanol and epicoprostanol found from body decomposition originates from released cholesterol rather than from the gut contents (not yet confirmed to be the case), it would be expected that human body decomposition coprostanol+epicoprostanol concentrations would be very much higher (>3 times) than 24-ethyl coprostanol+24-ethyl epicoprostanol concentrations. However, β-sitosterol concentrations were relatively high in some of the analysed samples (notably in sample 2). Because this compound is the source of 24-ethyl coprostanol and 24-ethyl epicoprostanol, bodies with high levels of β-sitosterol in the gut contents (suggested as coming from baby formula milk) could result in lower than expected coprostanol+epicoprostanol:24-ethyl coprostanol+24-ethyl epicoprostanol concentration ratios.

- ➢ The results of this series of tests cannot establish categorically whether the sewage facility was being used at the time when the human remains were deposited. It is a matter of historic record to establish when and how long the facility was used.
- ➢ The results of this series of tests cannot establish categorically whether the non-decomposed human remains had been deposited in the chambers, or whether the bodies have previously been stored (and decomposed) elsewhere, with mainly bones being placed in the chambers.

2.2 It is not possible to determine the extent to which the deposited human infant remains which are known to be present may have contributed to this, or to what extent human faecal material may also have done so.

2.3 The presence of VOC hotspots within the northern and western boundary samples but not the southern and eastern boundary samples is of note. A number of the hotspots for compounds characteristic of bone decomposition, particularly ketones, but also aliphatic alcohols and *n*-aldehydes, are found at locations with high bone densities.

2.4 However, the concentrations of the solid organic biomarkers in the analysed samples were very low, much lower than would be expected if the analysed material had entirely originated from human sewage waste.

2.5 The samples collected from the site boundaries (negative control samples; samples 55 and 57) had generally lower biomarker concentrations than the samples collected from within the chambers where remains were located.

2.6 10-Hydroxy stearic acid, cholesterol and the faecal stanols, coprostanol and epicoprostanol have been recognised as being products of the decomposition of mammalian remains (including human), and their concentration patterns generally differ from those of human sewage material. The presence of these compounds in the samples collected from the chambers could, at least in part, have come from decomposed human bodies.

2.7 The reasons for the low biomarker concentrations found in the samples are not easy to assess. If the chambers represented a closed cesspit or a number of cesspits, it is possible that the collected sewage had been removed before depositing the human cadaver material; soil may have been added at the same time, or soil may have seeped in from the roof area of the chambers. If there were one or more piped out flows (i.e. the facility was a septic tank, or was connected to a sewer outflow), it would be expected that little sewage would be left behind.

2.8 Samples 55 and 57 (west boundary and east boundary locations respectively) and sample 14 (no visible human remains) have different isotopic profiles to the other samples examined, reflecting possibly a lesser influence from human remains (or human sewage).

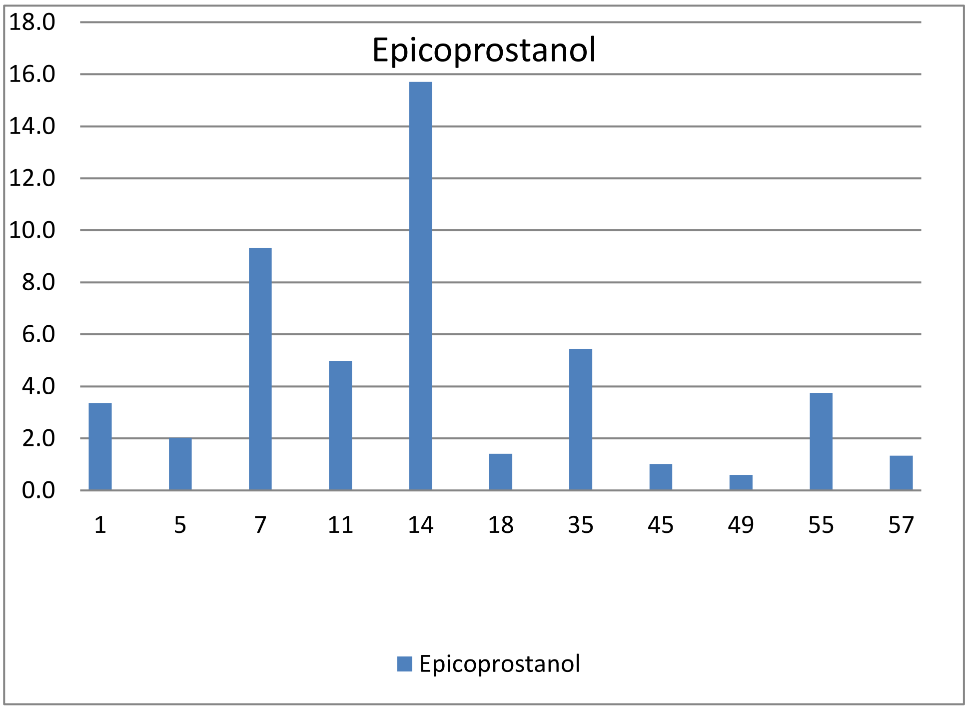
2.9 It is likely that some signature due to faecal material is present, but it is also likely that the human remains have also contributed to the signatures observed, and the presence of compounds associated with decomposition of bone at locations of high bone density in the samples is suggestive of this.

3. Further considerations on faecal markers and decomposition

3.1 Relative proportions of sterols and stanols (cholesterol, β-sitosterol, coprostanol, 24-ethylcoprostanol) indicate the faecal source (e.g. herbivores, omnivores, birds).
Coprostanol, epicoprostanol, 24-ethylcoprostanol and 24-ethyl-epicoprostanol originate from faeces **or** cadaver decomposition.

3.2 High levels of cholesterol, coprostanol and epicoprostanol are found in soils adjacent to, or underlying decomposing cadavers.

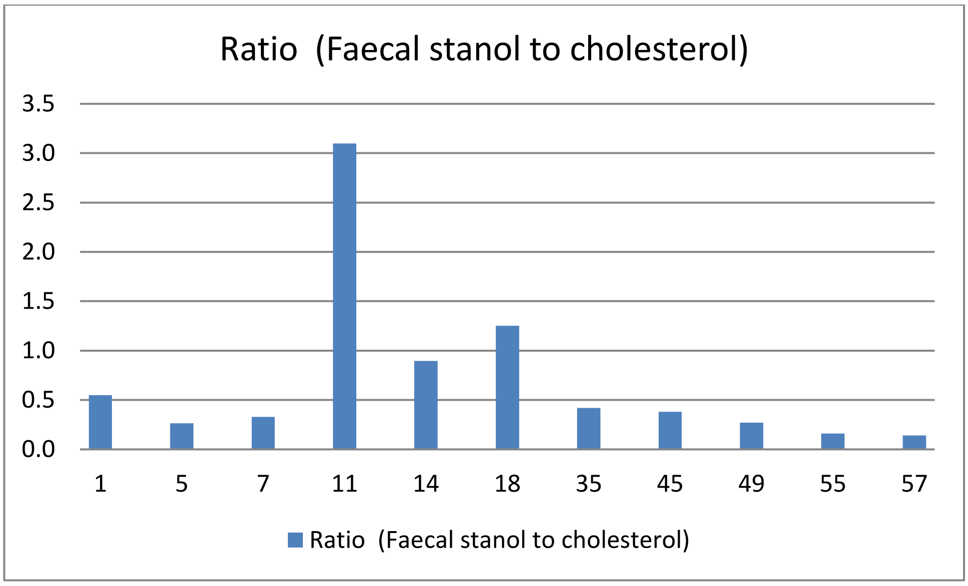
Figure 1 Concentration (mg/kg) of epicoprostanol in samples analysed for solid organic markers



3.3 Fresh faecal material typically has low levels of epicoprostanol and 24-ethylepicoprostanol compared with their respective isomers, coprostanol and 24-ethylcoprostanol, while old faecal sources have relatively high levels of the former compounds (epicoprostanol and 24-ethylepicoprostanol). It is not known whether cadaver decomposition over time has similarly changing levels of these compounds

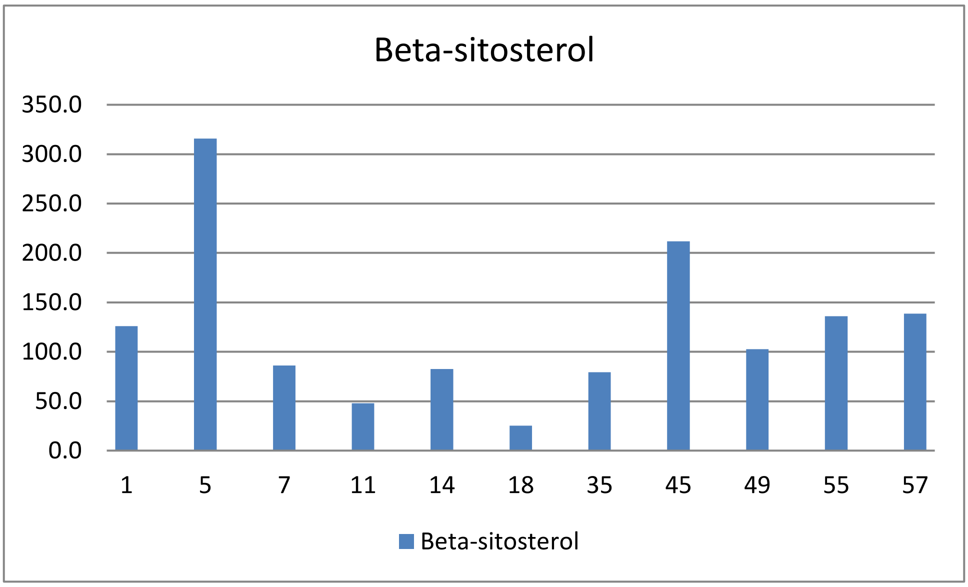
3.4 24-Ethylcoprostanol originates from sitosterol, whereas the 'epis' are associated with faecal age.

Figure 2. Ratio of faecal stanols (coprostanol and epicoprostanol) to cholesterol in samples analysed for solid organic markers.



3.5 Most of the analysed samples had relatively high concentrations of beta-sitosterol- higher than expected from cadaver decomposition, and higher than expected from human adults or children eating solid food. The reason for the relatively high betasitosterol concentrations are not clear, but it is possible that the source was faeces, or cadaver gut contents from infants receiving formula milk containing vegetable oils. However, the two external control samples also had relatively high values for beta-sitosterol, although this may have come from vegetation associated with these samples.

Figure 3. Beta-sitosterol concentration (mg/kg) in samples analysed for solid organic markers.



3.6 Possible strategy for initial further work would be:

1. to complete the analysis of all the samples for organics and isotopes to accompany the VOCs.

2. Select some appropriate sewage samples of different ages for VOC and isotope analysis.

Comments:

4.1 There are currently several issues which hamper detailed interpretation.

4.2 One is the considerable passage of the time since the potential use of the facility for storage of sewage, potential leaks into surrounding areas, and that so little is known of the history of use of that site.

4.3 A sampling issue is that the solid organics are very spatially distributed, and grab sampling may have introduced a high level of heterogeneity to the results. On direct contact sampling, samples can be collected at points directly under the torso of the skeleton to increase chances of obtaining compounds which are indicative of human decomposition. Previous research has shown that cholesterol can be recovered from soil directly underneath the torso, while none can be detected at the feet for example.

4.4 The other issue is that both the sewage storage and the decomposition has taken place more than 60 years ago and there is no direct experimental data (neither pig surrogate nor human decomposition studies) to predict what happens to compounds over that period of time.

4.5 Another issue is that not much knowledge is known about the actual history of these sites to give time lines of potential usage.

4.6 In addition, the negative control samples do not appear to represent no contact with sewage (e.g. Site 55 may have been in contact with sewage which had leaked at one point in time (per comm Niamh McC)).

4.7 In addition, some of the sites (e.g. Site 14) which had been reported not to have any visible remains may contain human sewage or remains.

4.8 The recovery of the human remains, quantification of numbers and age, along with careful spatial sampling with subsequent analysis of VOC, Organics and stable isotopic data of all collected samples, along with carefully selected and collected reference samples, would allow much improved interpretation.

Declaration

If you have any queries in relation to this report or any of the work that we have performed then please contact the laboratory.

Report provided by: Prof Lorna DAWSON, Dr Tom SHEPHERD and Dr Bob MAYES
Mrs Jasmine ROSS has quality checked this report.

Signature:

Signature:

Signature:

Address *The James Hutton Institute*
Aberdeen
AB15 8QH

Email: [*lorna.dawson@hutton.ac.uk*](mailto:lorna.dawson@hutton.ac.uk)

Telephone number: *01224 395328, mobile: 07815 178093*

Dated the 26 June 2017