'Tell me what you eat, and I will tell you who you are'

A Multi-Tissue and Multi-Scalar Isotopic Study of Diet and Mobility in Early Medieval England and its European Neighbours

Samantha Alicen Leggett

Volume II of II

Newnham College
University of Cambridge
August 2020

This dissertation is submitted for the degree of Doctor of Philosophy

Appendices

A Digital Appendices

See digital files on my Github page (see below) for data files (.csv and .xlsx) and R code. I have included my raw and cleaned data files from the mass spectrometers, as well as the collated databases (including my primary data). The digital appendices also include large size images such as the DDC cell maps in Chapter 8 which, and the original dendrograms which were too large to include in text at their full size/resolution.

Files available from: https://github.com/samleggs22/PhD_thesis

B Laboratory Standard Operations Procedures (SOPs)

These are copies of the Dorothy Garrod Laboratory SOPs and numbered in line with the overall list of protocols. There are also machine details and data interpretation/quality control notes included from both the Dorothy Garrod Laboratory and the Godwin Laboratory at the Department of Earth Sciences where the mass spectrometers are housed and run.

B.i SOP1 – Sampling Bone

LAB PROTOCOL #1 OCT 2009

SAMPLING BONE

Equipment
1. Appropriate drill & drill-bits
2. Extraction hood 1
3. Sandblaster
4. Pliers, hacksaw if necessary
5. Cutting block
6. Jeweller's small scales

Consumables
1. Glass test tubes
2. Tube racks
3. Plastic bags
4. Aluminium foil
5. Marker pens & biros

Personal Protective Equipment

Wear gloves and lab specs.

Protocol

This should all be carried out in the Wet Lab, basement of the Courtyard Building.
For combustion in the isotope mass spec, there must be **at least** 2-5mg of protein. To ensure sufficient protein after extraction, use approx 500 mg of bone, use more for older / worse-preserved bones.

Cutting bone pieces

ALL DRILLING AND CUTTING OF BONE TO BE DONE IN EXTRACTION HOOD 1
1. Choose a long bone if possible. Aim to sample mid-shaft.
2. Label small plastic bag with sample code of the bone you are cutting.
3. Fix diamond cutting wheel into drill, following instructions on the wall of the lab.
4. Put bone onto wooden chopping block in the extraction hood.
5. Cut off a piece using several cuts from each side.
6. Weigh on small scales to check that you have cut approx 0.5g. If not sufficient, cut off more.
7. Put sample into plastic bag.

Sandblasting

Sandblast bone following instructions on the wall beside the equipment.
Hold bone sample tightly in tweezers in non-dominant hand. Hold sandblaster nozzle in dominant hand, and work sand spray over the surface of the bone, ensuring that you take off any surface dirt from whole bone surface.

Crushing bone (***if necessary***)
1. Label glass test tube with sample code of the bone you are cutting.
2. Weigh labelled test tube to mg level (3dpl on balance) and record weight in lab book.
3. Crush bone using a percussion mortar, or hammer, aluminium foil and plastic bag.
4. Tip pieces into the test tube.
5. Weigh test tube + sample and record weight in lab book. [If you write down sample codes in yr lab book in a long list, and have 3 columns next to it, then you can have one column for empty test tube, one for tube + bone, then subtract one from the other, and record bone weight.]
6. Leave test tube rack covered with aluminium foil on the bench top.

The sample is now ready for acid treatment.

B.ii SOP1a – Sampling Bone in the Field

LAB PROTOCOL #1A — OCTOBER 2009

SAMPLING BONE & TOOTH IN THE FIELD

Equipment

1. Appropriate drill & drill-bits
   * battery-powered Dremel if no mains power
   * normal drill if mains power
2. Pliers, hacksaw if necessary
3. Cutting block
4. Jeweller's small scales

Consumables

5. Plastic bags
6. Aluminium foil
7. Tref tubes

Personal Protective Equipment

Wear gloves, face mask and lab specs.

Protocol

Cutting bone pieces

1. Choose a long bone if possible. Aim to sample mid-shaft.
2. Label small plastic bag with sample code of the bone you are cutting.
3. Fix diamond cutting wheel into drill.
4. Put bone onto wooden chopping block.
5. Cut off a piece using several cuts from each side.
6. Weigh on small scales to check that you have cut approx 0.5g. If not sufficient, cut off more.
7. Put sample into plastic bag.

Sampling teeth/shell

1. If necessary, clean shell/tooth with toothbrush to remove adhering material.
2. With a pointed tungsten drill bit, use the side of the drill bit to remove any cementum / tartar sticking to the surface of the enamel.
3. Label & weigh each micro-centrifuge tube.
4. Using a long rod shaped diamond drill bit collect power from shell/tooth sub sample onto a weighing paper. Don't get any dentine in sample. At very minimum 5.5mg of enamel is needed. Try to take at least 6 mg.

B.iii SOP3 – Collagen Extraction from Archaeological Bone using HCl

COLLAGEN EXTRACTION FROM ARCHAEOLOGICAL BONE USING HCL

Equipment
1. Sandblaster (if bone not powdered)
2. Centrifuge (if bone powdered)
3. Fridge
4. Oven @75°C
5. Freezers: -20°C & -80°C
6. Freeze-dryer

Chemicals
1. 0.5M aq. HCl (stored in fridge)
2. Distilled / Milli-Q water
3. pH 3 water

Consumables
1. Glass test tubes
2. Tube racks
3. Ezee filters
4. Plastic pop-on lids for test tubes
5. Pasteur pipettes
6. Plastic test tubes
7. 200ml glass beakers for pouring acid

Personal Protective Equipment
Wear lab coat and lab specs at all times.
Wear gloves when making up 0.5M acid.

Protocol
For combustion in the isotope mass spec, there must be **at least** 2-5mg of protein. To ensure sufficient protein after extraction, use approx 500 mg of bone, more for older / worse-preserved bones.

1. Cleaning:
If the sample is not powdered clean bones by sandblasting, ensuring that all ink is removed. Sandblast bone following instructions beside equipment.
Hold bone sample tightly in tweezers in non-dominant hand. Hold sandblaster nozzle in dominant hand, and work sand spray over the surface of the bone, ensuring that you take off any surface dirt from whole bone surface.
If necessary, crush bone using a percussion mortar, or hammer, aluminium foil and plastic bag.

2. Demineralisation:
Put bone chunks/powder into labelled & weighed 12ml glass test tubes. Record weights of bone used (i.e. weigh tube + sample after putting sample in tube).
For bone chunks, add approx. 8ml cold 0.5M HCl to test tube and cover over whole test tube rack with aluminium foil. Leave in the fridge for several days. Shake once/twice daily. Change acid every 2-4 days, by decanting off acid v slowly into waste beaker, being careful not to pour off bone pieces. If the bone is very fragmented, an ezee filter can be used, as shown by the supervisor. When sample is soft or floats, it is done: test by poking with Pasteur pipette. Decant off the supernatant liquor into a waste beaker, and discard it down the sink with excess water. Rinse in dist. water x3 (can use Ezee filters here).
For bone powder, add approx. 8ml cold 0.5M HCl to test tube and cover over whole test tube rack with aluminium foil. Leave on the bench top for 3hrs, shaking every half an hour. Change the acid, and leave on the benchtop overnight. In the morning, rinse in water x3 by the following method: centrifuge at 2000rpm for 10mins, then using Ezee filter, decant off & discard supernate (down the sink with excess water), then add water, then repeat x2.

3. Gelatinisation:
Gelatinise the remaining collagen pellet by heating in pH 3.0 water (about 7ml) at 75°C for 48 hours, by the following method. Add 8ml pH 3 water to tubes. Place in oven at 75°C, put plastic lid on each tube, then cover over all tops of tubes with tin foil, as demonstrated by supervisor. Ensure that the lids stay on as they have a tendency to 'pop off' when heated – use a pencil to push the lid down into the tube properly. Do not force it as you may crack the top of the tube. Check lids every morning/evening or when passing the lab. After 48hrs, all the collagen should have dissolved, leaving behind all acid insoluble material. Using an Ezee filter, filter off the

supernatant liquor into labelled ***pre-weighed*** plastic test tubes. This solution contains the collagen.

4. Freeze-drying:
Freeze the plastic tubes overnight at -20°C at a sharp angle (put racks at angle in the freezer) to increase surface area of the frozen solution. Transfer to -80°C freezer for 4hrs, then into the freeze-drier, following instructions given by Tamsin and as labelled on the freeze-drier. Leave for between 1& 4 days until dry. The freeze-dried material contains collagen and possibly some acid salts. Weigh tube+sample after drying and this will give you the yields of collagen.

B.iv SOP19 – Tooth Preparation Using Sodium Hypochlorite

LAB PROTOCOL #19 JULY 2010

TOOTH PREPARATION USING SODIUM HYPOCHLORITE

Equipment
1. Extraction hood 2
2. Vortex mixer
3. Fridge
4. Centrifuge

Chemicals
1. 2-3% aq. Sodium hypochlorite
2. 0.1M aq. Acetic acid

Consumables
1. Micro-centrifuge tubes
2. Drill & drill bits
3. Gilson pipettes & pipette tips

Personal Protective Equipment
Wear lab coat, lab specs and nitrile gloves at all times.

Protocol
Tooth enamel isotope protocol of Marie Balasse (CNRS Paris)

ALL DRILLING AND CUTTING OF TOOTH TO BE DONE IN EXTRACTION HOOD 2, IN THE WET LAB, BASEMENT OF THE COURTYARD BUILDING

For each batch of samples, you should also prepare 2 samples of Std 1 and 2 samples of Std 3, to allow us to assess that the pre-treatment has been carried out correctly. A batch is typically 18, so this would be 14 samples and 4 standards.

1. Clean tooth with toothbrush to remove adhering material. All non-EU sediment must be collected and placed in DEFRA bin. Surfaces must be wiped with a suitable disinfectant.
2. Use a drill bit to remove any cementum / tartar sticking to the surface of the enamel.
3. Label & weigh a micro-centrifuge tube for each sample.
4. Using a diamond drill bit collect power from tooth sub sample onto a weighing paper. Don't get any dentine in sample. At very minimum 5.5mg of enamel is needed. Try to take at least 6 mg.
5. If there are chunks of enamel in the sample then it will need sieving. Grind the sample in the agate pestle and mortar and sieve using the 90 micron sieve. Clean the sieve and pestle and mortar using methanol (not acetone) between samples. Any surplus sample can be kept as below.
6. Put sample into micro-centrifuge tube and weigh again to calculate amount of sample. The maximum that can be treated is 12mg. If you take more then weigh out a suitable aliquot and keep the rest in an Eppendorf with the sample in case you wish to analyse it again.
   For standards 1 and 3 weigh approx 6 mg of each.
   The samples can be left at this stage.
7. Add approximately 0.1ml per mg of sample of 2-3% aqueous sodium hypochlorite ($NaOCl$) to tubes and vortex mix them. Leave for 24 hours in the fridge (4°C). This removes all organic material.
8. Centrifuge tubes at 8000 rpm for 5 min, then decant liquid. Don't lose any powder; it is better to leave some liquid in the tube than run the risk of losing the powder.
9. Add distilled water to tube, vortex, then centrifuge tubes at 8000 rpm for 5 min. Gently tip off liquid retaining powder.
10. Repeat water rinse, vortex and centrifuge 4 more times (5 in total).
11. After final rinse use micro-pipette with disposable tip to remove any liquid still in tubes. Use a clean pipette tip for each sample.
12. Add approx 0.1ml per mg of sample of 0.1M aq. acetic acid. This will remove secondary carbonates. Vortex mix, then leave for 4 hours at room temperature.
13. Add distilled water to tube, vortex, then centrifuge tubes at 8000 rpm for 5 min. Gently tip off liquid.
14. Repeat water rinse, vortex and centrifuge 4 more times (5 in total).

15. After final rinse use micro-pipette with disposable tip to remove any liquid still in tubes. Use a clean pipette tip for each sample.
16. Freeze samples for 1 hour at -20°C.
17. Freeze dry samples for 1 hour 30 minutes.
18. Weigh tube+sample again to establish weight loss during pre-treatment. It is normal to lose 40 to 50% of sample weight during pre-treatment.

    Its currently recommended (July 2010) to send 2-4 mg of finished sample for analysis on the Gas Bench.

B.v EA-IRMS Mass Spectrometer Details

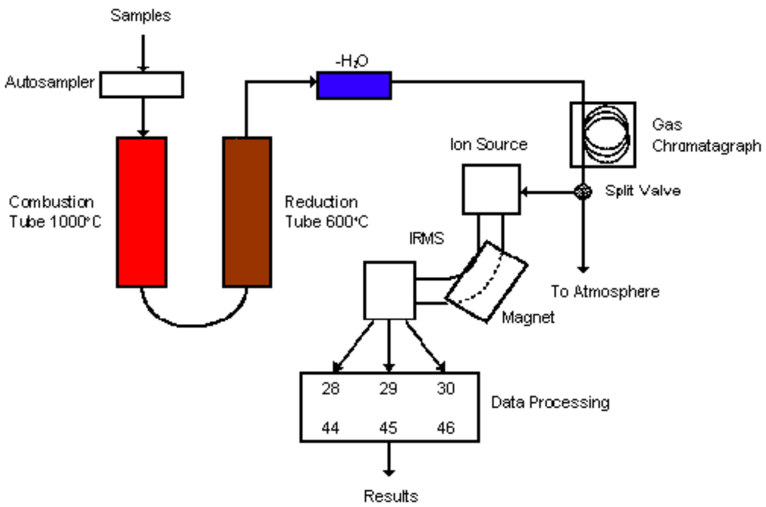
Isotope Analysis for C&N of organics at the Godwin Lab

Analyses are performed using an automated elemental analyzer coupled in continuous-flow mode to an isotope-ratio-monitoring mass-spectrometer (Costech elemental analyser coupled to a Finnigan Delta V mass spectrometer). Stable isotope concentrations are measured as the ratio of the heavier isotope to the lighter isotope relative to an internationally defined scale, VPDB for carbon, and AIR for nitrogen (Hoefs 1997). Isotopic results are reported as δ values ($\delta^{13}C$ and $\delta^{15}N$) in parts per 1000 or 'permil' (‰) values, where $\delta^{15}N_{AIR} = [(^{15/14}N_{sample} / ^{15/14}N_{AIR}) - 1] \times 1000$. Based on replicate analyses of international and laboratory standards, measurement errors are less than ±0.2‰ for $\delta^{13}C$ and $\delta^{15}N$. The isotopic standards used are: IAEA standard of caffeine for carbon and nitrogen; in-house laboratory standards of nylon, alanine, protein 2 and EMC (Elemental Microanalysis caffeine) standard for carbon, nitrogen and atomic C/N ratios.

Hoefs, J. (1997) Stable Isotope Geochemistry, Berlin, Springer.

In your thesis, please put in an acknowledgement to James Rolfe, Godwin Lab, Dept of Earth Sciences, for help with isotopic analyses, and to Catherine Kneale for help in sample preparation and analysis.

Schematic diagram
(courtesy of T.C. O'Connell)



Costech ECS 4010 - Valencia, CA, USA
Delta V – Bremen, Germany

B.vi Gas-bench Mass Spectrometer Details

Isotope Analysis for C&O of carbonates at the Godwin Lab

Balasse method

Enamel powder was treated for bioapatite extraction as described in Balasse et al. (2002). Briefly, enamel was treated with sodium hypochlorite 2–3% (24 h) to remove organic matter, and then with 0.1 M acetic acid (4 h, 0.1 ml/mg) to remove exogenous carbonate. The samples were then freeze dried overnight. The vials were sealed with a screw cap holding a septa and PCTFE washer to make a vacuum seal, and the samples reacted with 100% orthophosphoric acid at 90°C using a Gas Bench II coupled to a Delta V mass spectrometer for isotopic analysis. Results are reported with reference to the international standard VPDB calibrated through the NBS19 standard (Coplen. 1995; Hoefs 1997) and the precision is better than ±0.08‰ for $^{13}C/^{12}C$ and better than ±0.10‰ for $^{18}O/^{16}O$.

Balasse, M., Ambrose, S. H., Smith, A. B. & Price, T. D. (2002). The seasonal mobility model for prehistoric herders in the south-western Cape of South Africa assessed by isotopic analysis of sheep tooth enamel. J. Archaeol. Sci. 29: 917–932.
Coplen, T.B., New IUPAC guidelines for the reporting of stable hydrogen, carbon and oxygen isotope-ratio data. Journal of Research of the National Institute of Standards and Technology 100, 285-285, 1995
Hoefs, J. (1997) Stable Isotope Geochemistry, Berlin, Springer.

Godwin method

Samples were transferred in to glass vials and soaked in approximately 0.5ml of a 3% aqueous solution of hydrogen peroxide for 30 min. Acetone (analytical grade) was added and the sample ultrasonicated for 30 seconds, and the liquid carefully decanted off using a tissue. The samples were then dried in an oven at 50 degrees Centigrade overnight. The vials were sealed with a screw cap holding a septa and PCTFE washer to make a vacuum seal, and the samples reacted with 100% orthophosphoric acid at 90°C using a Micromass Multicarb Sample Preparation System. The carbon dioxide produced was dried and transferred cryogenically into a Gas Bench II coupled to a Delta V mass spectrometer for isotopic analysis. Results are reported with reference to the international standard VPDB calibrated through the NBS19 standard (Coplen. 1995; Hoefs 1997) and the precision is better than ±0.08‰ for $^{13}C/^{12}C$ and better than ±0.10‰ for $^{18}O/^{16}O$.

Coplen, T.B., New IUPAC guidelines for the reporting of stable hydrogen, carbon and oxygen isotope-ratio data. Journal of Research of the National Institute of Standards and Technology 100, 285-285, 1995
Hoefs, J. (1997) Stable Isotope Geochemistry, Berlin, Springer.

Acknowledgements

Please put in an acknowledgement to James Rolfe, Godwin Lab, Dept of Earth Sciences, for help with isotopic analysis, and to Catherine Kneale for help in sample preparation and analysis

B.vii EA-IRMS Data Interpretation Notes 1

GODWIN LAB, UNIVERSITY OF CAMBRIDGE **JUNE 2018**

C & N ISOTOPIC ANALYSIS **DATA INTERPRETATION**

The results

OR How to look at isotope data from ea-irms – a novice's guide

The output comes as an excel file. The file will be called a date such as "05june08.xls". You need to remember this name, since if you lose all your data, then you can ask for a copy of it. If you do forget the file name, then we will be able to track it down, but it will take more time.
There is one data sheet for the carbon, and one for the nitrogen results. If Catherine has been very kind, she may have amalgamated them onto one sheet. If not, then you need to get all the data onto one sheet, bearing in mind that not all samples run contain both carbon and nitrogen, so be sure to match the sample names up.

Output files

The carbon isotope results sheet

Identifier 1	Identifier 2	Date	Time	FileHeader: Filename	Line	Type	Amount	Rt	Area All	Ampl 44	Amt%	d 13C/12C
Nylon		06/05/08	15:08:28	Nylon__-0000.cf	2	Start Reference Mean	0.77	261.9	299.613	12397	62.10	-26.51
Nylon		06/05/08	15:18:20	Nylon__-0001.cf	3	Add Reference Mean	0.83	262.3	282.813	11696	62.10	-26.45
Alanine		06/05/08	15:28:12	Alanine__-0001.cf	4	Sample	0.85	264.4	152.719	6391	31.39	-26.98
Alanine		06/05/08	15:38:04	Alanine__-0002.cf	5	Sample	0.7	264.8	151.794	6365	37.88	-27.04
Oxalic		06/05/08	15:47:55	Oxalic__-0002.cf	6	Sample	1.64	264.4	169.957	7133	18.10	-18.81
GM02	c	06/05/08	15:57:47	GM02_c_-0002.cf	7	Sample	0.9	266.9	145.688	5672	28.28	-15.51
GM04	c	06/05/08	16:07:39	GM04_c_-0002.cf	8	Sample	0.84	266.3	188.957	7524	39.30	-19.34
GM05	c	06/05/08	16:17:31	GM05_c_-0002.cf	9	Sample	0.68	269.2	113.906	4481	29.26	-18.43
GM07	c	06/05/08	16:27:23	GM07_c_-0002.cf	10	Sample	0.71	266.1	150.81	6024	37.11	-19.88

The nitrogen isotope results sheet

Identifier 1	Identifier 2	Date	Time	FileHeader: Filename	Line	Type	Amount	Rt	Area All	Ampl 28	Amt%	d 15N/14N
Nylon		06/05/08	15:08:28	Nylon__-0000.cf	2	Start Reference Mean	0.77	152.6	156.816	6277	12.10	-1.51
Nylon		06/05/08	15:18:20	Nylon__-0001.cf	3	Add Reference Mean	0.83	153.2	146.691	5921	12.10	-1.65
Alanine		06/05/08	15:28:12	Alanine__-0001.cf	4	Sample	0.85	152.4	162.58	6448	12.23	-1.54
Alanine		06/05/08	15:38:04	Alanine__-0002.cf	5	Sample	0.7	151.9	161.838	6419	14.78	-1.55
GM02	c	06/05/08	15:57:47	GM02_c_-0002.cf	7	Sample	0.9	153.2	140.268	5283	9.97	18.78
GM04	c	06/05/08	16:07:39	GM04_c_-0002.cf	8	Sample	0.84	153.4	174.522	6728	13.28	12.84
GM05	c	06/05/08	16:17:31	GM05_c_-0002.cf	9	Sample	0.68	154.9	108.336	4049	10.19	12.82
GM07	c	06/05/08	16:27:23	GM07_c_-0002.cf	10	Sample	0.71	152.2	146.374	5605	13.18	11.76

If the data has been amalgamated onto one sheet, then it will look something like this.

Identifier 1	Identifier 2	Date	Time	FileHeader: I	Line	Type	Amount	Area All	Ampl 44	Amt%	d 13C/12C	Area All	Ampl 28	Amt%	d 15N/14N
NYLON		04/15/08	11:04:55	NYLON__-0	3	Start Reference	0.80	288.25	11004	62.10	-26.15	152.86	5634	12.10	-1.92
NYLON		04/15/08	11:14:06	NYLON__-0	4	Add Reference I	0.65	243.58	9271	62.10	-26.20	129.70	4720	12.10	-1.93
ALANINE		04/15/08	11:23:18	ALANINE__-	5	Sample	0.79	188.31	7191	40.03	-26.88	202.66	7387	15.90	-1.69
ALANINE		04/15/08	11:32:29	ALANINE__-	6	Sample	0.87	203.25	7733	39.23	-26.87	219.20	8018	15.62	-1.66
SB66	a	04/15/08	11:41:42	SB66_a_-0(	7	Sample	0.72	126.34	4687	29.47	-20.61	125.63	4435	10.82	8.95
SB73	a	04/15/08	11:50:52	SB73_a_-0(	8	Sample	0.87	235.91	8764	45.54	-19.26	237.92	8618	16.95	9.79
SB77	a	04/15/08	12:00:04	SB77_a_-0(	9	Sample	0.79	216.72	8031	46.07	-20.00	219.06	7891	17.19	9.86
SB93	a	04/15/08	12:09:14	SB93_a_-0(	10	Sample	0.79	164.18	5789	34.90	-19.66	163.63	5654	12.84	9.18
SB94	a	04/15/08	12:18:25	SB94_a_-0(	11	Sample	0.85	176.29	6159	34.83	-19.34	174.72	6007	12.74	7.77
SB95	a	04/15/08	12:27:36	SB95_a_-0(	12	Sample	0.87	238.70	8683	46.07	-18.85	238.35	8504	16.98	9.75
SB130	a	04/15/08	12:36:47	SB130_a_-(	13	Sample	0.83	252.31	9251	51.05	-20.13	253.72	9147	18.95	9.94

There are extra columns that are no use to you, but you need to keep all the raw data on one sheet, and copy it onto another sheet to play with it – that way, if you make a mistake, then you have the raw data to go back to.

The column headings mean this:

Identifier 1	Your sample code
Identifier 2	Your replicate code (a, b, c etc)
Date	The date it was run
Time	The time it was run
FileHeader: Filename	The individual raw data file name for that sample analysis
Line	The number that the sample was run in the run-list
Type	Whether it was a std (usual) or a reference (the nylon samples)
Amount	The amt in mg that you weighed out
Area All	The area of the carbon peak
Ampl 44	The amplitude (height) of the carbon peak
Amt%	The percentage of carbon in the sample, calculated from the weight of the sample, relative to the nylon samples that you included
d 13C/12C	$\delta^{13}C$
Area All	The area of the nitrogen peak
Ampl 28	The amplitude (height) of the nitrogen peak
Amt%	The percentage of nitrogen in the sample, calculated from the weight of the sample, relative to the nylon samples that you included
d 15N/14N	$\delta^{15}N$

You will need to add a column for the C/N ratio (see later for the formula).

How to say if it is good data

There is a list of rules to follow when you get your data. You cannot just look at it and say if you like the numbers or not without checking if it is good quality data.
You must check this for each and every run, before amalgamating data from running samples in triplicate.

1. Make sure mass spec was working OK
   Laboratory stds and unknowns must be close (±0.1‰) to the expected value. If the means are not close to these values, then the data may need re-processing or re-analysing. You should check with Catherine or Tamsin.

	$\delta^{15}N$ (‰)	$\delta^{13}C$ (‰)	C/N (see later)
Caffeine	+1.0(+1.1)	-27.5	2.0
USGS-40	-4.5	-26.2	5.0
Alanine	-1.4	-26.9	3.0 (finished March 2018)
New Nylon	-3.14	-26.55	6.0 (δ values are not consistent – ignore)
Protein 2	+6.0	-26.9/-27.0	4.0
EMC	-2.5/-2.6	-35.8/-35.9	2.0
New Alanine	-23.88	-1.22	3.0

The $\delta^{13}C$ and $\delta^{15}N$ values of the New Nylon are not very consistent – don't worry. We primarily use this as a size standard to calculate the percentage C and N of your samples.

2. Check size of samples
   Amplitude of C&N peaks of the samples should be within half to double of the amplitude of the reference gas peaks, the closer the better. These are tuned to be the same as the amplitude of the alanine peaks. So look at the alanine peak (typically 6000-7000mV), and then calculate if your sample peaks are within half to double (typically 3000-13,000mV).
   If they are outside this range, then they are too small or too large, and will need reweighing (either more or less). See Catherine.

3. Are the samples OK in terms of protein composition?
   i.e. is your atomic C/N OK?
   This calculated value is an indicator of the quality of the protein combusted.
   It is more an issue for collagen that has been extracted in the lab, or other protein samples.
   The C/N of bone is 2.9-3.6 (theoretical is 3.17). Outside this range, you have not got collagen (or have got corrupted collagen) so cannot use the data.
   The C/N of hair keratin is about 3.0-3.8 (theoretical is 3.4), and again, outside that range you have to forget that data.
   If you are analysing anything else, such as soils or plants, these may be highly variable, and the C/N ratio cannot be used to exclude data. However, bear in mind that the mass spec is set up to run samples with a C/N of 3, so if you are running anything else, then you will have to double-check that both your carbon and nitrogen data is within the range of the reference peak (see point 2), thus that your data is OK.

   The ratio is calculated as **(Amt % C / Amt % N)** × **(14/12)**, which gives you an **atomic ratio** (ratio of number of C atoms to number of N atoms in the sample). You need to calculate this for your samples and stds in the results file.

4. Does your collagen have enough C & N in it?
   You can find this out from the calculated % of C&N in the results file.

Collagen	modern	acceptable
% C:	40-50%	>13%
% N:	14-18%N	>4-5%

   If your percentage values look very odd (too high), this may be an artefact of the machine, or may be due to inaccuracies in weighing. If in doubt, consult Catherine or Tamsin.

If all of the above are OK, you can use the data.

Combining data from multiple runs

For multiple runs, get each run lined up with all the other
- KEEP each data run separate (label sheet with run file name, usually a date)
  - You need to save this raw data in case you do anything wrong, and need to recover it, and so you can pull out any odd ones when doing the comparison (see below)
- Make an extra sheet on which you can amalgamate all data
- Copy and paste the replicates isotope data, lining them all up correctly (see below).
- Make a series of columns at the far right
  - mean, std dev, and no of analyses for each of d13C, d15N, C/N ratio (see above)
- Calculate these values for each sample.
- Look for any odd ones, i.e. where the std dev is larger than about 0.2, and then check
  - why it is odd – which replicate is different, is anything wrong with it?

if you cannot find out which is odd and why, then you may need to reweigh the sample for re-analysis

A very small version of what the amalgamated file of multiple replicates looks like:

Identifier 1	Run file	Amount (mg Aliquot a	Amt % C Aliquot a	d13C Aliquot a	Amt % N Aliquot a	d15N Aliquot a	C/N ratio Aliquot a
nylon	11may06	2.10	66.0	-26.4	11.4	-1.5	
nylon	11may06	0.96	62.1	-26.5	12.1	-1.4	5.99
nylon	11may06	0.87	62.1	-26.5	12.1	-1.4	5.99
alanine	11may06	0.63	39.3	-26.9	15.6	-1.2	2.94
alanine	11may06	0.85	40.2	-27.0	16.1	-1.2	2.92
400B	11may06	0.80	45.3	-19.4	17.0	10.2	3.12
364B	11may06	0.70	39.6	-19.3	14.1	8.5	3.29
136B	11may06	0.90	52.5	-19.3	19.7	8.4	3.11
121B	11may06	0.90	35.5	-19.5	13.5	8.5	3.08
100B	11may06	0.60	78.9	-19.6	29.3	7.7	3.14
51B	11may06	0.60	34.9	-19.8	13.0	8.3	3.14
T51A	11may06	0.80	38.9	-20.0	14.2	8.6	3.20
T51B	11may06	0.70	50.9	-20.0	18.7	8.7	3.18
collagen_std	11may06	0.90	53.2	-23.0	20.4	6.2	3.05
137B	11may06	0.80	35.7	-19.6	13.3	6.5	3.13
203B	11may06	0.90	52.2	-19.3	19.6	8.4	3.11
337B	11may06	0.70	54.3	-19.6	20.3	8.2	3.12
A+	11may06	1.00	39.2	-22.9	14.9	6.1	3.07
B+	11may06	0.90	37.8	-22.9	14.4	6.0	3.06
351	11may06	0.70	36.9	-19.3	14.3	8.6	3.02
303	11may06	0.90	58.6	-19.2	22.5	10.7	3.05
118	11may06	1.00	50.4	-19.3	19.1	8.4	3.07
365A	11may06	0.70	45.1	-19.7	17.0	8.3	3.10
389B	11may06	0.70	36.1	-19.5	13.5	6.6	3.12
113	11may06	0.90	36.6	-19.5	13.7	8.4	3.12
393	11may06	0.60	49.2	-19.7	18.4	8.5	3.12
361	11may06	0.70	41.5	-19.0	15.6	11.1	3.11

Identifier 1	Run file	Amount (mg Aliquot b	Amt % C Aliquot b	d13C Aliquot b	Amt % N Aliquot b	d15N Aliquot b	C/N ratio Aliquot b
nylon	12may06	2.21	64.4	-26.5	12.6	-1.5	
nylon	12may06	0.94	62.1	-26.5	12.1	-1.4	5.99
nylon	12may06	0.69	62.1	-26.4	12.1	-1.5	5.99
alanine	12may06	0.90	40.2	-27.0	15.6	-1.2	3.00
alanine	12may06	0.80	40.5	-27.0	15.7	-1.2	3.00
400B	12may06	0.80	49.1	-19.3	18.0	10.1	3.17
364B	12may06	0.70	52.7	-19.2	18.7	8.6	3.29
136B	12may06	0.70	55.4	-19.3	20.3	8.3	3.18
121B	12may06	0.80	39.0	-19.2	14.4	8.5	3.16
100B	12may06	0.60	54.4	-19.3	19.8	7.5	3.21
51B	12may06	0.60	72.1	-20.0	25.8	8.9	3.26
T51A	12may06	0.70	38.4	-20.0	13.6	8.5	3.30
T51B	12may06	1.00	49.1	-20.0	17.7	8.8	3.23
collagen_std	12may06	0.80	59.3	-23.0	22.2	6.1	3.11
137B	12may06	0.80	47.3	-19.6	17.2	6.7	3.21
203B	12may06	0.60	55.0	-19.3	20.2	8.2	3.17
337B	12may06	0.90	49.1	-19.5	18.0	8.3	3.18
A+	12may06	0.90	53.8	-22.9	20.0	6.1	3.13
B+	12may06	1.00	54.0	-23.0	20.1	6.2	3.13
351	12may06	0.70	47.5	-19.4	17.8	8.8	3.11
303	12may06	0.80	50.8	-19.1	19.0	10.6	3.12
118	12may06	0.90	45.6	-19.1	16.9	8.3	3.15
365A	12may06	1.00	37.9	-19.7	13.9	8.4	3.17
389B	12may06	0.80	37.7	-19.4	13.8	6.7	3.18
113	12may06	1.00	47.4	-19.6	17.4	8.5	3.18
393	12may06	0.60	32.0	-19.6	11.5	8.1	3.25
361	12may06	0.70	55.1	-19.1	20.2	11.3	3.19

Identifier 1	Run file	Amount (mg Aliquot c	Amt % C Aliquot c	d13C Aliquot c	Amt % N Aliquot c	d15N Aliquot c	C/N ratio Aliquot c
nylon	13may06	2.22	63.0	-26.5	12.2	-1.5	6.02
nylon	13may06	0.83	62.1	-26.5	12.1	-1.4	5.99
nylon	13may06	0.76	62.1	-26.6	12.1	-1.5	5.99
alanine	13may06						
alanine	13may06						
400B	13may06	0.80	36.9	-19.2	14.2	9.8	3.04
364B	13may06	0.70	73.2	-19.1	26.8	8.8	3.19
136B	13may06	0.90	42.6	-19.2	16.3	8.3	3.05
121B	13may06	0.80	42.9	-19.5	16.5	8.4	3.04
100B	13may06	0.60	98.8	-19.5	37.4	7.7	3.08
51B	13may06	0.60	73.8	-20.0	27.5	8.8	3.13
T51A	13may06	0.70	57.7	-19.9	21.4	8.6	3.14
T51B	13may06	0.80	47.6	-20.0	17.9	8.5	3.10
collagen_std	13may06	0.80	51.6	-22.9	20.2	6.0	2.99
137B	13may06	0.70	64.6	-19.7	24.4	6.7	3.09
203B	13may06	0.90	65.2	-19.4	24.8	8.4	3.06
337B	13may06	0.80	54.0	-19.6	20.7	8.2	3.05
A+	13may06	0.80	62.9	-23.0	24.4	6.1	3.01
B+	13may06	0.80	67.7	-23.0	25.7	6.2	3.08
351	13may06	0.70	43.9	-19.4	17.2	8.6	2.98
303	13may06	0.90	33.6	-19.1	13.1	10.3	3.00
118	13may06	0.70	46.4	-19.2	17.9	8.1	3.02
365A	13may06	1.00	33.1	-19.7	12.6	8.2	3.06
389B	13may06	0.70	33.6	-19.5	12.9	6.4	3.04
113	13may06	0.90	46.3	-19.5	17.7	8.4	3.06
393	13may06	0.70	41.4	-19.7	15.9	8.3	3.04
361	13may06	0.70	44.0	-19.0	16.9	11.0	3.04

Identifier 1	mean d13C	Std dev C	Reps-C	Mean d15N	Std dev N	Reps-N	Mean C/N
nylon			3	-1.5	0.0	3	
nylon	-26.5	0.0	3	-1.4	0.0	3	5.99
nylon	-26.5	0.1	3	-1.4	0.0	3	5.99
alanine			2			2	
alanine			2			2	
400B	-19.3	0.1	3	10.0	0.2	3	3.11
364B	-19.2	0.1	3	8.6	0.2	3	3.25
136B	-19.3	0.0	3	8.3	0.1	3	3.11
121B	-19.4	0.2	3	8.5	0.0	3	3.09
100B	-19.5	0.1	3	7.6	0.1	3	3.14
51B	-20.0	0.1	3	8.7	0.3	3	3.18
T51A	-20.0	0.1	3	8.6	0.1	3	3.22
T51B	-20.0	0.0	3	8.7	0.1	3	3.17
collagen_std	-23.0	0.0	3	6.1	0.1	3	3.05
137B	-19.6	0.0	3	6.6	0.1	3	3.14
203B	-19.3	0.1	3	8.4	0.1	3	3.11
337B	-19.6	0.1	3	8.2	0.0	3	3.11
A+	-22.9	0.0	3	6.1	0.0	3	3.07
B+	-23.0	0.0	3	6.1	0.1	3	3.09
351	-19.4	0.0	3	8.7	0.1	3	3.03
303	-19.1	0.0	3	10.5	0.2	3	3.05
118	-19.2	0.1	3	8.3	0.2	3	3.08
365A	-19.7	0.0	3	8.3	0.1	3	3.11
389B	-19.5	0.0	3	6.6	0.1	3	3.12
113	-19.5	0.0	3	8.5	0.1	3	3.12
393	-19.7	0.0	3	8.3	0.2	3	3.14
361	-19.1	0.1	3	11.1	0.1	3	3.11

It is MUCH easier to line the replicates up side by side than attempt to arrange them one after another, firstly for looking at the overall results, and secondly for copying and pasting this 'data summary' into another sheet for actually plotting etc.

What the series of columns at the far right (mean, std dev, and no of analyses (Reps-N) for each of d13C, d15N, C/N ratio) looks like:

Identifier 1	mean d13C	Std dev C	Reps-C	Mean d15N	Std dev N	Reps-N	Mean C/N
nylon			3	-1.5	0.0	3	
nylon	-26.5	0.0	3	-1.4	0.0	3	5.99
nylon	-26.5	0.1	3	-1.4	0.0	3	5.99
alanine			2			2	
alanine			2			2	
400B	-19.3	0.1	3	10.0	0.2	3	3.11
364B	-19.2	0.1	3	8.6	0.2	3	3.25
136B	-19.3	0.0	3	8.3	0.1	3	3.11
121B	-19.4	0.2	3	8.5	0.0	3	3.09
100B	-19.5	0.1	3	7.6	0.1	3	3.14
51B	-20.0	0.1	3	8.7	0.3	3	3.18
T51A	-20.0	0.1	3	8.6	0.1	3	3.22
T51B	-20.0	0.0	3	8.7	0.1	3	3.17
collagen_std	-23.0	0.0	3	6.1	0.1	3	3.05
137B	-19.6	0.0	3	6.6	0.1	3	3.14
203B	-19.3	0.1	3	8.4	0.1	3	3.11
337B	-19.6	0.1	3	8.2	0.0	3	3.11
A+	-22.9	0.0	3	6.1	0.0	3	3.07
B+	-23.0	0.0	3	6.1	0.1	3	3.09
351	-19.4	0.0	3	8.7	0.1	3	3.03
303	-19.1	0.0	3	10.5	0.2	3	3.05
118	-19.2	0.1	3	8.3	0.2	3	3.08
365A	-19.7	0.0	3	8.3	0.1	3	3.11
389B	-19.5	0.0	3	6.6	0.1	3	3.12
113	-19.5	0.0	3	8.5	0.1	3	3.12
393	-19.7	0.0	3	8.3	0.2	3	3.14
361	-19.1	0.1	3	11.1	0.1	3	3.11

A good std dev is ±0.2‰. Acceptable is ±0.3‰. In that case, you should look to see why the std dev is bigger – is one value 'out'? If yes, then try to work out why it is 'out'. If in doubt, consult Catherine/Tamsin. This data summary is what you should use as the values for all your calculations.

Errors

Generally, the machine error is of the order of ±0.1 to 0.2‰ for both $\delta^{13}C$ and $\delta^{15}N$. If you would like to know what the error is for the overall period (couple of weeks) during which your samples are run, then contact Catherine or Tamsin.

Machine Spec

If you want the full details of the machine spec and how it works for quoting in theses or papers, see the downloadable sheet on the website "EA_mass_spec_details.pdf" or contact Catherine or Tamsin.

GODWIN LAB, UNIVERSITY OF CAMBRIDGE **JULY 2008**
C & N ISOTOPIC ANALYSIS **DATA INTERPRETATION 2**

What to do with your results when you are happy with them

OR How to make nice plots and interpretations for your thesis and papers

Creating a "data summary" sheet

So you have your sheet of multiple runs (usually triplicate) of your samples, all side by side.
A very small version of what the amalgamated file of multiple replicates looks like:

Identifier 1	Run file	Amount (mg Aliquot a	Amt % C Aliquot a	d13C Aliquot a	Amt % N Aliquot a	d15N Aliquot a	C/N ratio Aliquot a
nylon	11may06	2.10	66.0	-26.4	11.4	-1.5	
nylon	11may06	0.96	62.1	-26.5	12.1	-1.4	5.99
nylon	11may06	0.87	62.1	-26.5	12.1	-1.4	5.99
alanine	11may06	0.63	39.3	-26.9	15.6	-1.2	2.94
alanine	11may06	0.85	40.2	-27.0	16.1	-1.2	2.92
400B	11may06	0.80	45.3	-19.4	17.0	10.2	3.12
364B	11may06	0.70	39.6	-19.3	14.1	8.5	3.29
136B	11may06	0.90	52.5	-19.3	19.7	8.4	3.11
121B	11may06	0.90	35.5	-19.5	13.5	8.5	3.08
100B	11may06	0.60	78.9	-19.6	29.3	7.7	3.14
51B	11may06	0.60	34.9	-19.8	13.0	8.3	3.14
T51A	11may06	0.80	38.9	-20.0	14.2	8.6	3.20
T51B	11may06	0.70	50.9	-20.0	18.7	8.7	3.18
collagen_std	11may06	0.90	53.2	-23.0	20.4	6.2	3.05
137B	11may06	0.80	35.7	-19.6	13.3	6.5	3.13
203B	11may06	0.90	52.2	-19.3	19.6	8.4	3.11
337B	11may06	0.70	54.3	-19.6	20.3	8.2	3.12
A+	11may06	1.00	39.2	-22.9	14.9	6.1	3.07
B+	11may06	0.90	37.8	-22.9	14.4	6.0	3.06
351	11may06	0.70	36.9	-19.3	14.3	8.6	3.02
303	11may06	0.90	58.6	-19.2	22.5	10.7	3.05
118	11may06	1.00	50.4	-19.3	19.1	8.4	3.07
365A	11may06	0.70	45.1	-19.7	17.0	8.3	3.10
389B	11may06	0.70	36.1	-19.5	13.5	6.6	3.12
113	11may06	0.90	36.6	-19.5	13.7	8.4	3.12
393	11may06	0.60	49.2	-19.7	18.4	8.5	3.12
361	11may06	0.70	41.5	-19.0	15.6	11.1	3.11

Identifier 1	Run file	Amount (mg Aliquot b	Amt % C Aliquot b	d13C Aliquot b	Amt % N Aliquot b	d15N Aliquot b	C/N ratio Aliquot b
nylon	12may06	2.21	64.4	-26.5	12.6	-1.5	
nylon	12may06	0.94	62.1	-26.5	12.1	-1.4	5.99
nylon	12may06	0.69	62.1	-26.4	12.1	-1.5	5.99
alanine	12may06	0.90	40.2	-27.0	15.6	-1.2	3.00
alanine	12may06	0.80	40.5	-27.0	15.7	-1.2	3.00
400B	12may06	0.80	49.1	-19.3	18.0	10.1	3.17
364B	12may06	0.70	52.7	-19.2	18.7	8.6	3.29
136B	12may06	0.70	55.4	-19.3	20.3	8.3	3.18
121B	12may06	0.80	39.0	-19.2	14.4	8.5	3.16
100B	12may06	0.60	54.4	-19.3	19.8	7.5	3.21
51B	12may06	0.60	72.1	-20.0	25.8	8.9	3.26
T51A	12may06	0.70	38.4	-20.0	13.6	8.5	3.30
T51B	12may06	1.00	49.1	-20.0	17.7	8.8	3.23
collagen_std	12may06	0.80	59.3	-23.0	22.2	6.1	3.11
137B	12may06	0.80	47.3	-19.6	17.2	6.7	3.21
203B	12may06	0.60	55.0	-19.3	20.2	8.2	3.17
337B	12may06	0.90	49.1	-19.5	18.0	8.3	3.18
A+	12may06	0.90	53.8	-22.9	20.0	6.1	3.13
B+	12may06	1.00	54.0	-23.0	20.1	6.2	3.13
351	12may06	0.70	47.5	-19.4	17.8	8.8	3.11
303	12may06	0.80	50.8	-19.1	19.0	10.6	3.12
118	12may06	0.90	45.6	-19.1	16.9	8.3	3.15
365A	12may06	1.00	37.9	-19.7	13.9	8.4	3.17
389B	12may06	0.80	37.7	-19.4	13.8	6.7	3.18
113	12may06	1.00	47.4	-19.6	17.4	8.5	3.18
393	12may06	0.60	32.0	-19.6	11.5	8.1	3.25
361	12may06	0.70	55.1	-19.1	20.2	11.3	3.19

Identifier 1	Run file	Amount (mg Aliquot c	Amt % C Aliquot c	d13C Aliquot c	Amt % N Aliquot c	d15N Aliquot c	C/N ratio Aliquot c
nylon	13may06	2.22	63.0	-26.5	12.2	-1.5	6.02
nylon	13may06	0.83	62.1	-26.5	12.1	-1.4	5.99
nylon	13may06	0.76	62.1	-26.6	12.1	-1.5	5.99
alanine	13may06						
alanine	13may06						
400B	13may06	0.80	36.9	-19.2	14.2	9.8	3.04
364B	13may06	0.70	73.2	-19.1	26.8	8.8	3.19
136B	13may06	0.90	42.6	-19.2	16.3	8.3	3.05
121B	13may06	0.80	42.9	-19.5	16.5	8.4	3.04
100B	13may06	0.60	98.8	-19.5	37.4	7.7	3.08
51B	13may06	0.60	73.8	-20.0	27.5	8.8	3.13
T51A	13may06	0.70	57.7	-19.9	21.4	8.6	3.14
T51B	13may06	0.80	47.6	-20.0	17.9	8.5	3.10
collagen_std	13may06	0.80	51.6	-22.9	20.2	6.0	2.99
137B	13may06	0.70	64.6	-19.7	24.4	6.7	3.09
203B	13may06	0.90	65.2	-19.4	24.8	8.4	3.06
337B	13may06	0.80	54.0	-19.6	20.7	8.2	3.05
A+	13may06	0.80	62.9	-23.0	24.4	6.1	3.01
B+	13may06	0.80	67.7	-23.0	25.7	6.2	3.08
351	13may06	0.70	43.9	-19.4	17.2	8.6	2.98
303	13may06	0.90	33.6	-19.1	13.1	10.3	3.00
118	13may06	0.70	46.4	-19.2	17.9	8.1	3.02
365A	13may06	1.00	33.1	-19.7	12.6	8.2	3.06
389B	13may06	0.70	33.6	-19.5	12.9	6.4	3.04
113	13may06	0.90	46.3	-19.5	17.7	8.4	3.06
393	13may06	0.70	41.4	-19.7	15.9	8.3	3.04
361	13may06	0.70	44.0	-19.0	16.9	11.0	3.04

Identifier 1	mean d13C	Std dev C	Reps-C	Mean d15N	Std dev N	Reps-N	Mean C/N
nylon			3	-1.5	0.0	3	
nylon	-26.5	0.0	3	-1.4	0.0	3	5.99
nylon	-26.5	0.1	3	-1.4	0.0	3	5.99
alanine			2			2	
alanine			2			2	
400B	-19.3	0.1	3	10.0	0.2	3	3.11
364B	-19.2	0.1	3	8.6	0.2	3	3.25
136B	-19.3	0.0	3	8.3	0.1	3	3.11
121B	-19.4	0.2	3	8.5	0.0	3	3.09
100B	-19.5	0.1	3	7.6	0.1	3	3.14
51B	-20.0	0.1	3	8.7	0.3	3	3.18
T51A	-20.0	0.1	3	8.6	0.1	3	3.22
T51B	-20.0	0.0	3	8.7	0.1	3	3.17
collagen_std	-23.0	0.0	3	6.1	0.1	3	3.05
137B	-19.6	0.0	3	6.6	0.1	3	3.14
203B	-19.3	0.1	3	8.4	0.1	3	3.11
337B	-19.6	0.1	3	8.2	0.0	3	3.11
A+	-22.9	0.0	3	6.1	0.0	3	3.07
B+	-23.0	0.0	3	6.1	0.1	3	3.09
351	-19.4	0.0	3	8.7	0.1	3	3.03
303	-19.1	0.0	3	10.5	0.2	3	3.05
118	-19.2	0.1	3	8.3	0.2	3	3.08
365A	-19.7	0.0	3	8.3	0.1	3	3.11
389B	-19.5	0.0	3	6.6	0.1	3	3.12
113	-19.5	0.0	3	8.5	0.1	3	3.12
393	-19.7	0.0	3	8.3	0.2	3	3.14
361	-19.1	0.1	3	11.1	0.1	3	3.11

At the far right-hand-side, you have a series of summary columns that should look like this (except that the Identifier 1 details are in Column A on the LHS):

Identifier 1	mean d13C	Std dev C	Reps-C	Mean d15N	Std dev N	Reps-N	Mean C/N
nylon			3	-1.5	0.0	3	
nylon	-26.5	0.0	3	-1.4	0.0	3	5.99
nylon	-26.5	0.1	3	-1.4	0.0	3	5.99
alanine			2			2	
alanine			2			2	
400B	-19.3	0.1	3	10.0	0.2	3	3.11
364B	-19.2	0.1	3	8.6	0.2	3	3.25
136B	-19.3	0.0	3	8.3	0.1	3	3.11
121B	-19.4	0.2	3	8.5	0.0	3	3.09
100B	-19.5	0.1	3	7.6	0.1	3	3.14
51B	-20.0	0.1	3	8.7	0.3	3	3.18
T51A	-20.0	0.1	3	8.6	0.1	3	3.22
T51B	-20.0	0.0	3	8.7	0.1	3	3.17
collagen_std	-23.0	0.0	3	6.1	0.1	3	3.05
137B	-19.6	0.0	3	6.6	0.1	3	3.14
203B	-19.3	0.1	3	8.4	0.1	3	3.11
337B	-19.6	0.1	3	8.2	0.0	3	3.11
A+	-22.9	0.0	3	6.1	0.0	3	3.07
B+	-23.0	0.0	3	6.1	0.1	3	3.09
351	-19.4	0.0	3	8.7	0.1	3	3.03
303	-19.1	0.0	3	10.5	0.2	3	3.05
118	-19.2	0.1	3	8.3	0.2	3	3.08
365A	-19.7	0.0	3	8.3	0.1	3	3.11
389B	-19.5	0.0	3	6.6	0.1	3	3.12
113	-19.5	0.0	3	8.5	0.1	3	3.12
393	-19.7	0.0	3	8.3	0.2	3	3.14
361	-19.1	0.1	3	11.1	0.1	3	3.11

This data summary is what you should use as the values for all your calculations.

You should leave your huge sheet of multiple analyses alone, and copy JUST the summary data onto another sheet to play with.

- Highlight the columns of interest (the summary ones, plus of course your sample codes which are likely to be in Column A – you may have to do this in two goes).
- Copy them

- Go into an empty sheet in your workbook and choose “Edit/Paste Special”, and click on the option “Values” then say “OK”. [This avoids problems with the fact that this summary is derived from a whole lot of equations.]

Combining archaeological and isotope data

Onto that summary data sheet, you should also add all the archaeological data that you have for your individual samples. This will vary depending on your project, but could include such information as:

- Grave / feature code
- Species
- Material type (bone, shell, tooth etc)
- Bone type (femur, rib etc)
- Sex
- Age
- Grave goods (presence/absence/details)
- Burial type

Basically as much information as you have can be included, as this is the sheet that you will use as a basis for your interrogation of the data.

You may end up with something that looks like this:

Grave No.	Feature No..	Skeleton No.	Age	Sex	pathology	stature (m)	non-metric trait	orientation	depth of grave			Rib				
											Reps	mean d13C	Std dev C	Mean d15N	Std dev N	Mean C/N
G1	17	51	older juvenile (10-12yrs)	?	enamel hyperplasias	-		W-E	0.24m		3	-20.3	0.1	10.6	0.0	3.2
G10	10	25	young adult	female	non observed	1.73	septal aperture (r)	W-E	0.04m		3	-19.8	0.5	11.8	0.0	3.1
G11	12	38	middle/mature adult	female	calculus, AMTL, OA in spine	1.65		W-E	0.16m		3	-20.3	0.0	11.7	0.0	3.1
G12	18	54	younger middle adult	male	calculus, fractured l. clavicle, degenerative joint disease of spine	1.69	septal aperture (bilateral)	W-E	0.20m		3	-20.2	0.1	12.2	0.0	3.1
G13	16	48	older middle adult	?male	calculus ,degenerative joint disease in lower spine	1.7		SW-NE	0.05m		3	-20.9	0.2	12.3	0.0	3.2
G14	13	39	younger middle adult	male	degenerative disease in lower spine	-	metopic suture retained	W-E	0.10m		3	-20.3	0.0	11.3	0.0	3.1
G15	15	42	young adult	male	degenerative joint disease in thoracic vertebrae	-	septal aperture (r)	W-E	0.04m		3	-20.2	0.1	11.1	0.0	3.2
G2	8	45	older subadult, (15-17 years)	?female	calculus, cribra orbitalia	1.61	septal aperture (bilateral)	SW-NE	0.12m		3	-21.0	0.0	12.3	0.0	3.2
G3	11	28	older subadult, (c.14-16 yrs)	?	enamel hyperplasias, calculus	-		W-E	0.16m		3	-20.3	0.1	12.7	0.0	3.2
G4	14	36	young adult	?	non observed	-		WNW-ESE	0.04m		3	-20.1	0.4	12.6	0.0	3.1

Plotting your archaeological and isotope data

Now comes the fun bit – start playing with your data.
The classic first charts to plot are:

- All your data, $\delta^{13}C$ vs $\delta^{15}N$

Then, depending on your project, it could be:

- All your data by species (if you have animals and humans), $\delta^{13}C$ vs $\delta^{15}N$
- All your human data by sex (if you have osteological or typological sex), $\delta^{13}C$ vs $\delta^{15}N$
- All your human data by age (if you have osteological age), $\delta^{13}C$ vs $\delta^{15}N$
- All your data by chronological period, $\delta^{13}C$ vs $\delta^{15}N$
- Mean + std dev for groups on the same chart, $\delta^{13}C$ vs $\delta^{15}N$
  if you need help with this, then either go on an Excel course (ideally you will have done this already, or ask one fo the isotope group VERY nicely. They will help you, but will not do it for you.

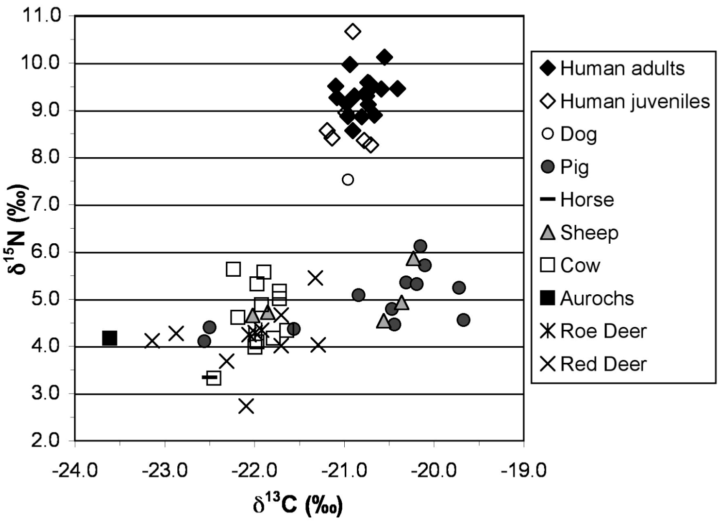
You can use

- x-y scatter plots for $\delta^{13}C$ vs $\delta^{15}N$

- line charts (Excel-speak) for plotting either $\delta^{13}C$ or $\delta^{15}N$ against categorical data (e.g. age classes or burial types)
- box & whisker plots (SPSS etc) for plotting mean +std dev for one variable against categorical data
- histograms / bar charts for frequencies of bins of $\delta^{13}C$ or $\delta^{15}N$ (but remember that $\delta^{13}C$ and $\delta^{15}N$ are numerical linear data so don't go well with a histogram).

Try to make your charts clear and simple.
Remember that legends should be obvious and readable.
Try to make it black + white, as easier for printing. If using colour, be careful of using ones that are hard to see, such as yellow.
Try to be consistent between charts, i.e. always pick the same symbol for one species or for one sex, and make sure that axes are consistent in scale.
Get rid of the default Excel grey background – it uses up toner and looks horrid.
Make sure your axes have an appropriate scale, are clear and legible.

Here's a good example:



Statistical tests on your archaeological and isotope data

You should need to do some statistical tests on your data to test relationships that you see, e.g. males look different to females in $\delta^{13}C$, or pigs from one period look different to pigs from another period in $\delta^{15}N$.
You can do this using SPSS or Sigmaplot or any other stats package. Look on the PWF for available programs. Excel is not great for stats, so avoid it. However, most packages will let you paste your data from Excel into them, meaning you can reformat your data in Excel, as this is often the easiest way to start.
Make sure you know what you are doing, and that you choose your test appropriately, e.g t-tests are only OK if your data are normally distributed (that means having a large enough data set).

Make sure you know how to report your data in the text (giving enough information to the reader that they can be sure that you did the test appropriately, and not too much that it is clear that you are writing down everything that the program gave you as output.).

Common tests we use are

- independent t-tests (if normal) for two groups
- paired t-tests (if normal) for two groups with matching data
- ANOVA (usually with a post-hoc Bonferroni correction) for more than two groups
- Mann-Whitney (& variants) if not normal.
- Kolmogorov-Smirnoff to test for normality
- Levene's test for equality of variance

Ask for help if you are stuck. But please ask for help at the Computing Services for practical "How do I?" questions, rather than take up a lot of time of one of the Isotope Gang.

Always make sure that the test you are doing can be related to something archaeologically relevant – almost no point in testing differences that have no relevance to your archaeological project.
Also ensure that you are not testing an "artefact" of the way you have categorised the data etc. Well, that could be interesting, but only if you recognise that it is an "artefact" or artifical construct, and not necessarily something meaningful.

C q-q plots: tests for Normality

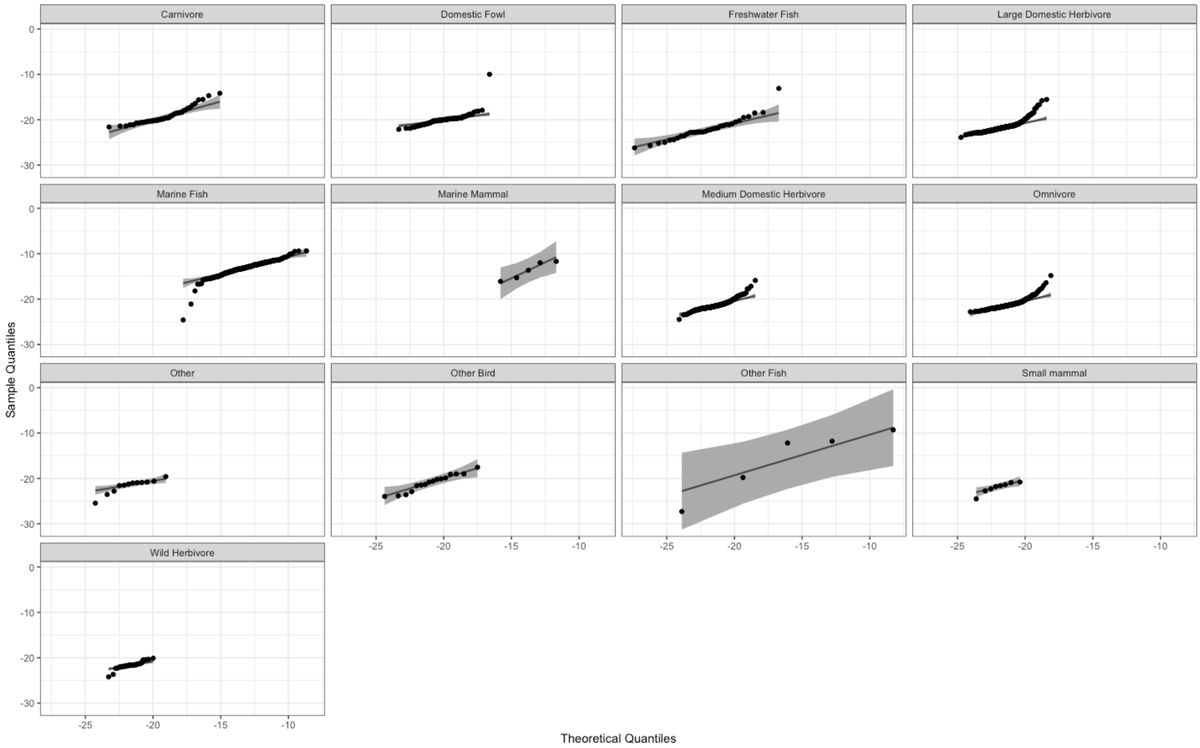


Figure C-1: q-q plots for all European faunal bone δ¹³C values by species group.

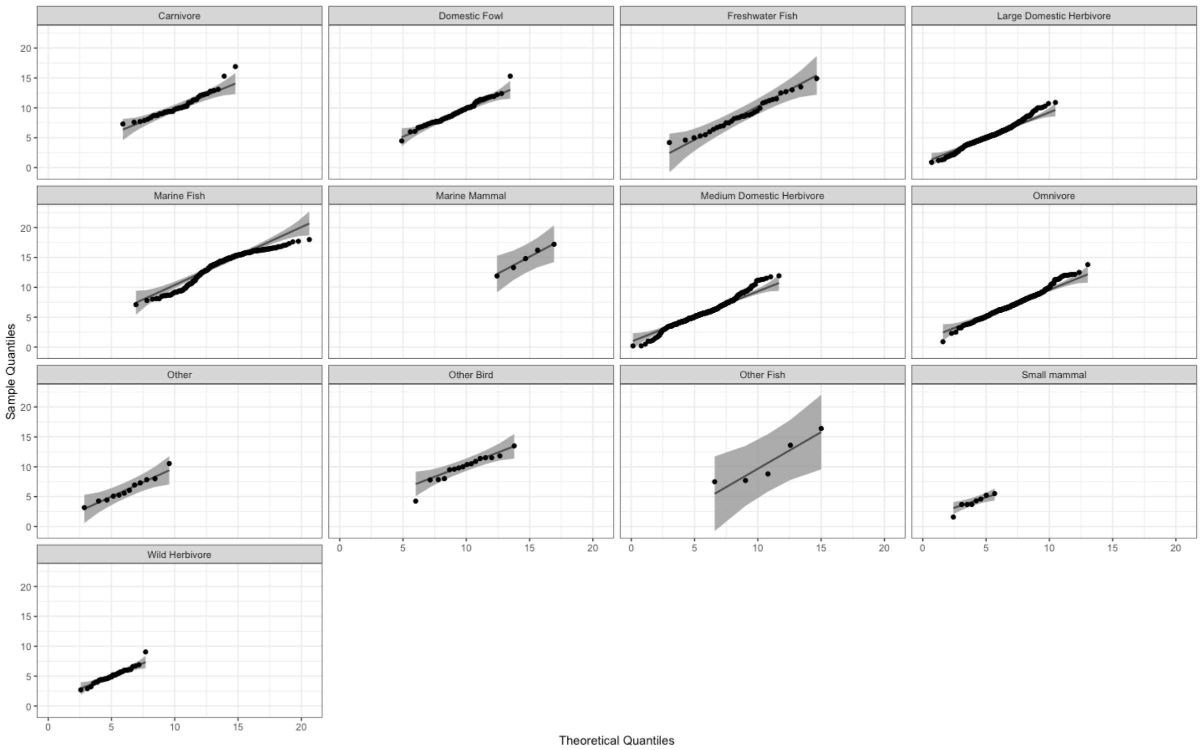


Figure C-2: q-q plots for all European faunal bone δ¹⁵N values by species group.

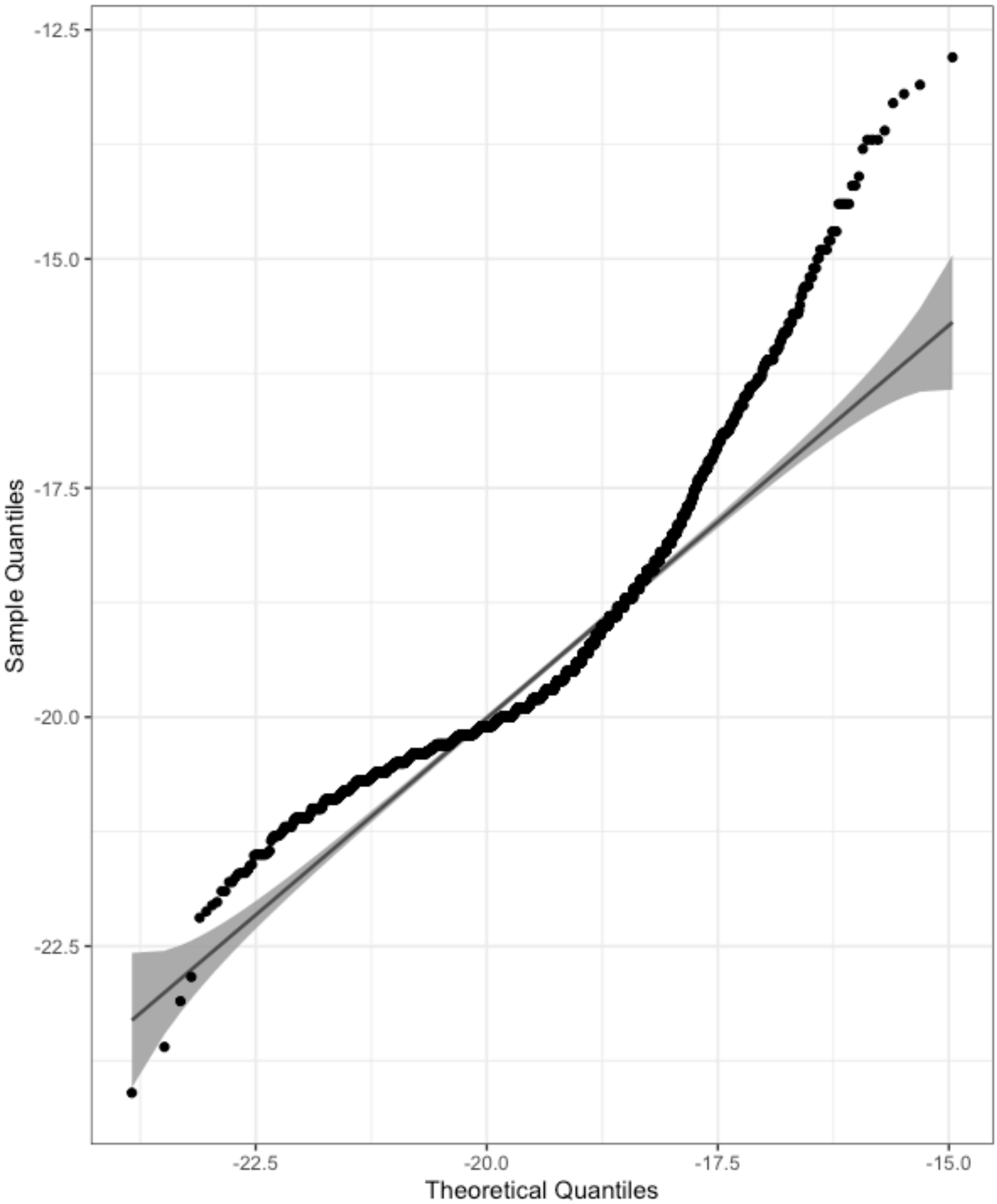


Figure C-3: q-q plot for bone $\delta^{13}C$ values in the whole human European dataset.

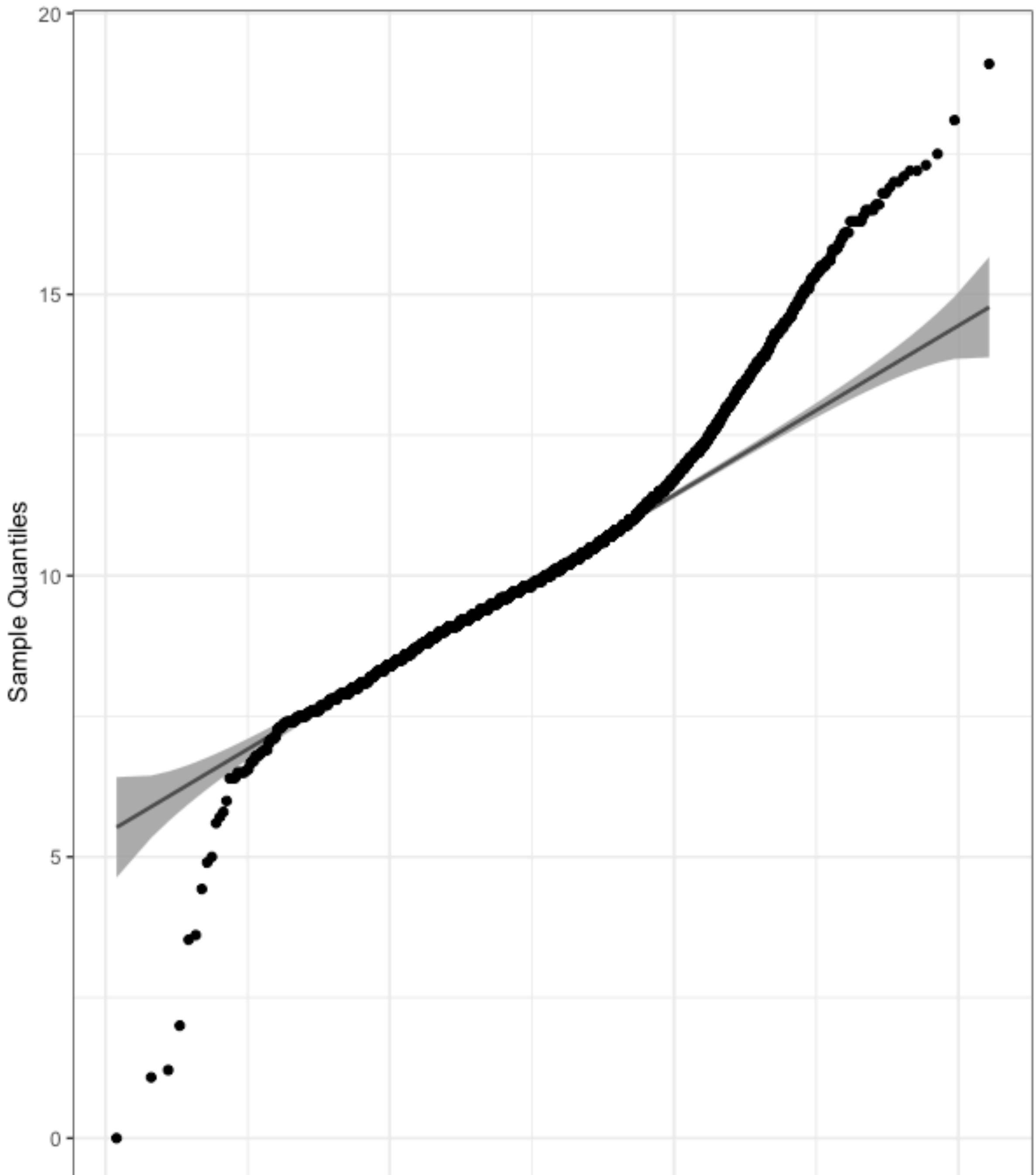


Figure C-4: q-q plot for bone $\delta^{15}N$ values in the whole human European dataset.

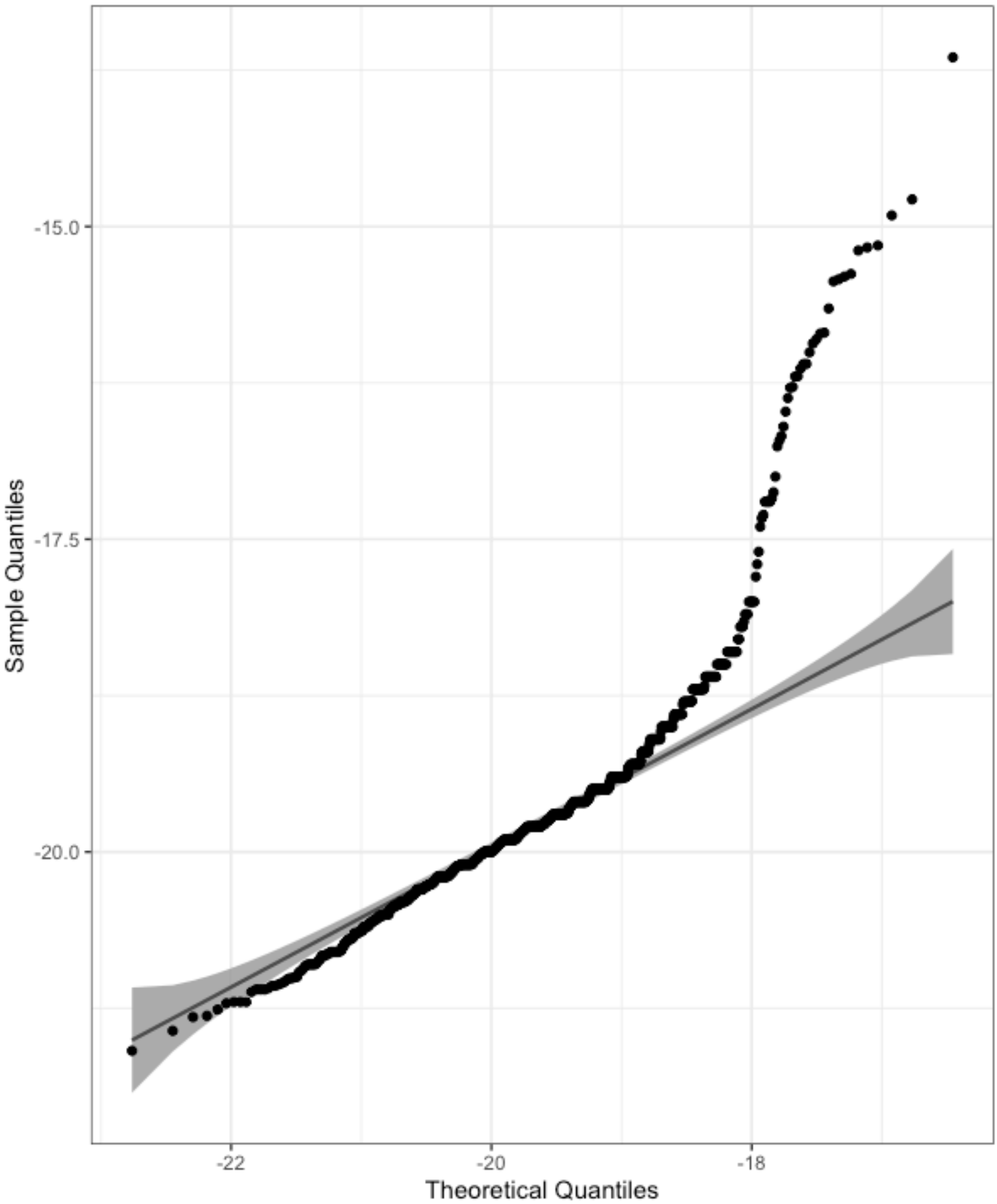


Figure C-5: q-q plot for dentine $\delta^{13}C$ values in the whole human European dataset.

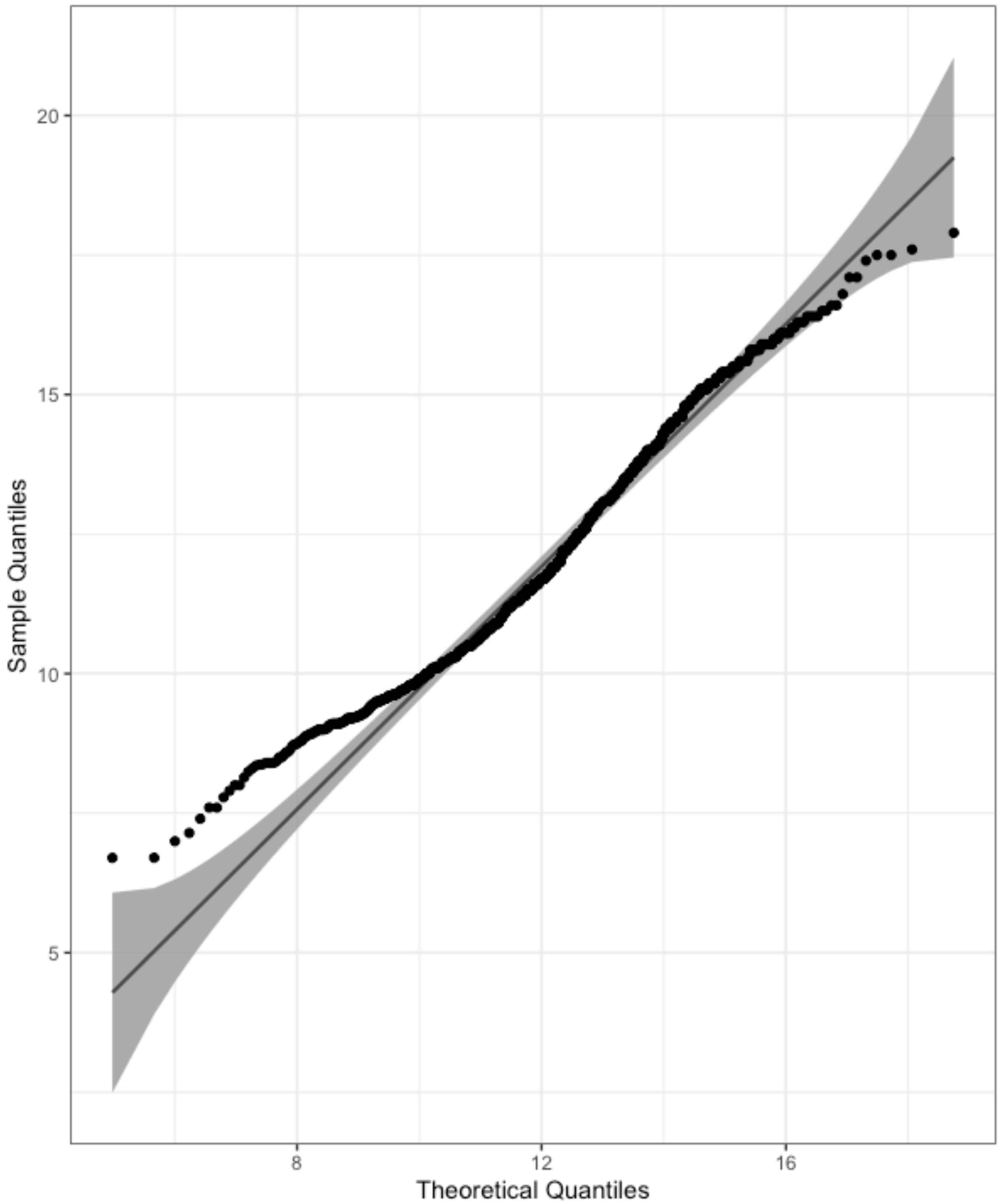


Figure C-6: q-q plot for dentine $\delta^{15}N$ values in the whole human European dataset.

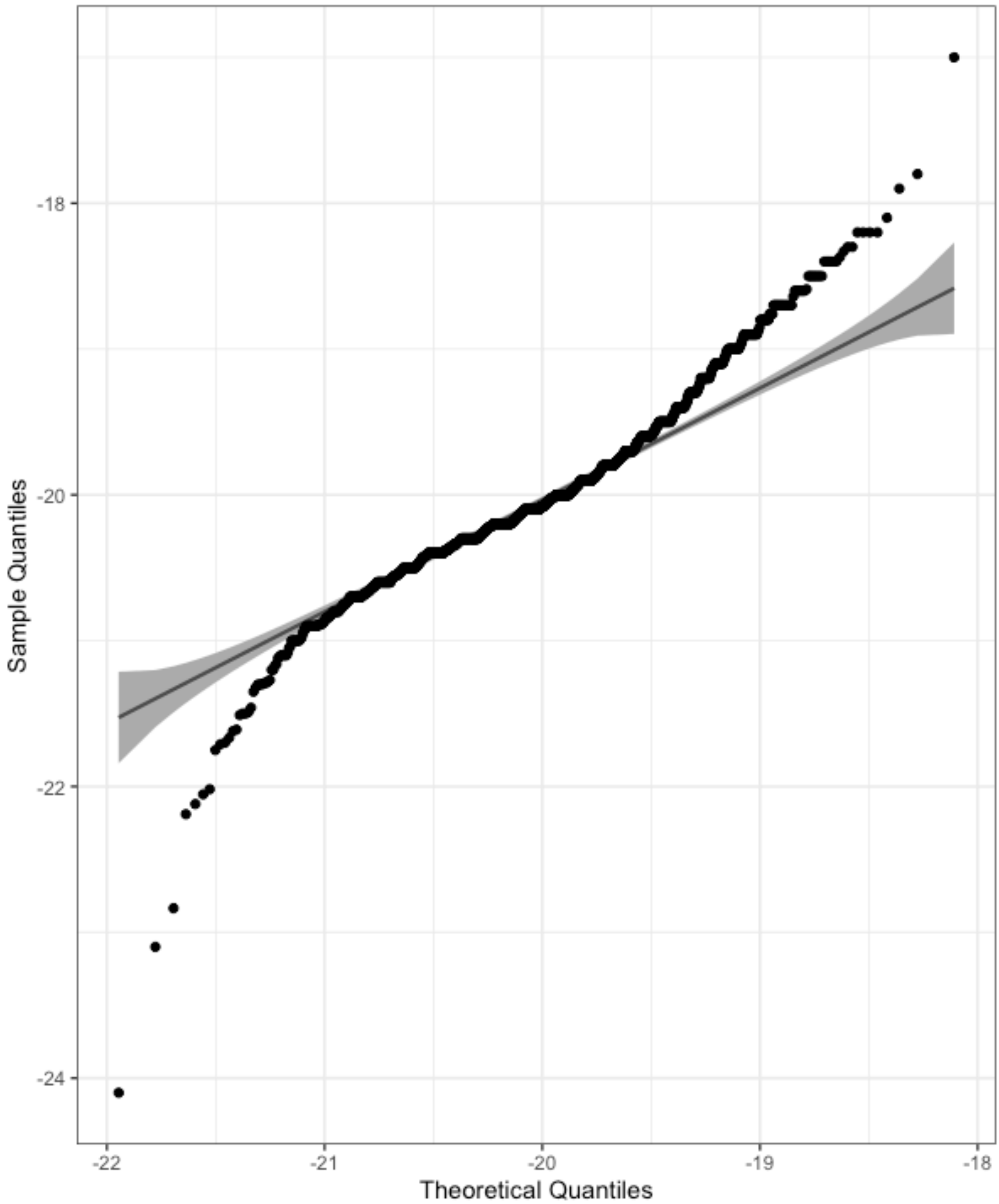


Figure C-7: q-q plot for bone δ[13]C values in the whole human England dataset.

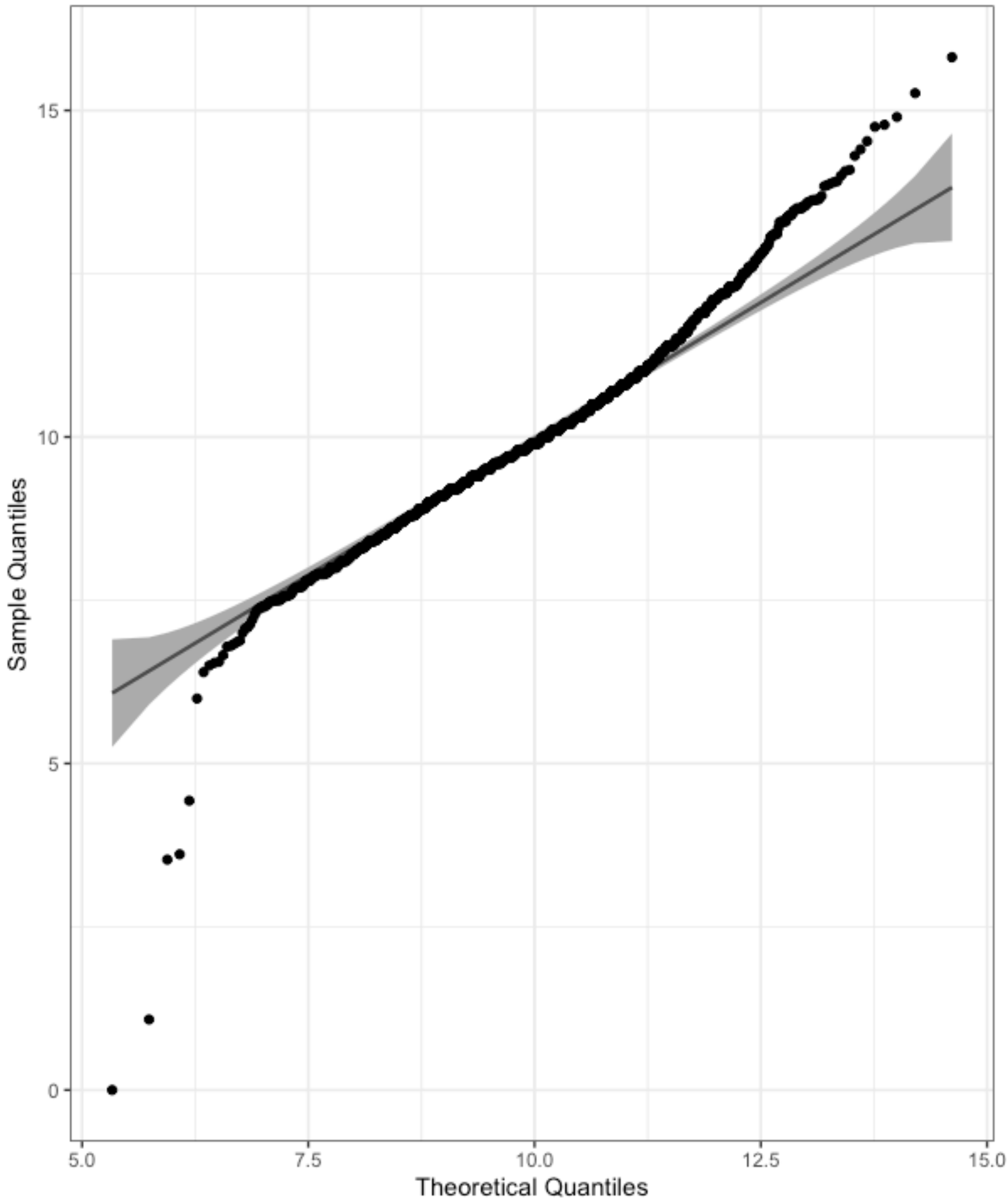


Figure C-8: q-q plot for bone δ¹⁵N values in the whole human England dataset.

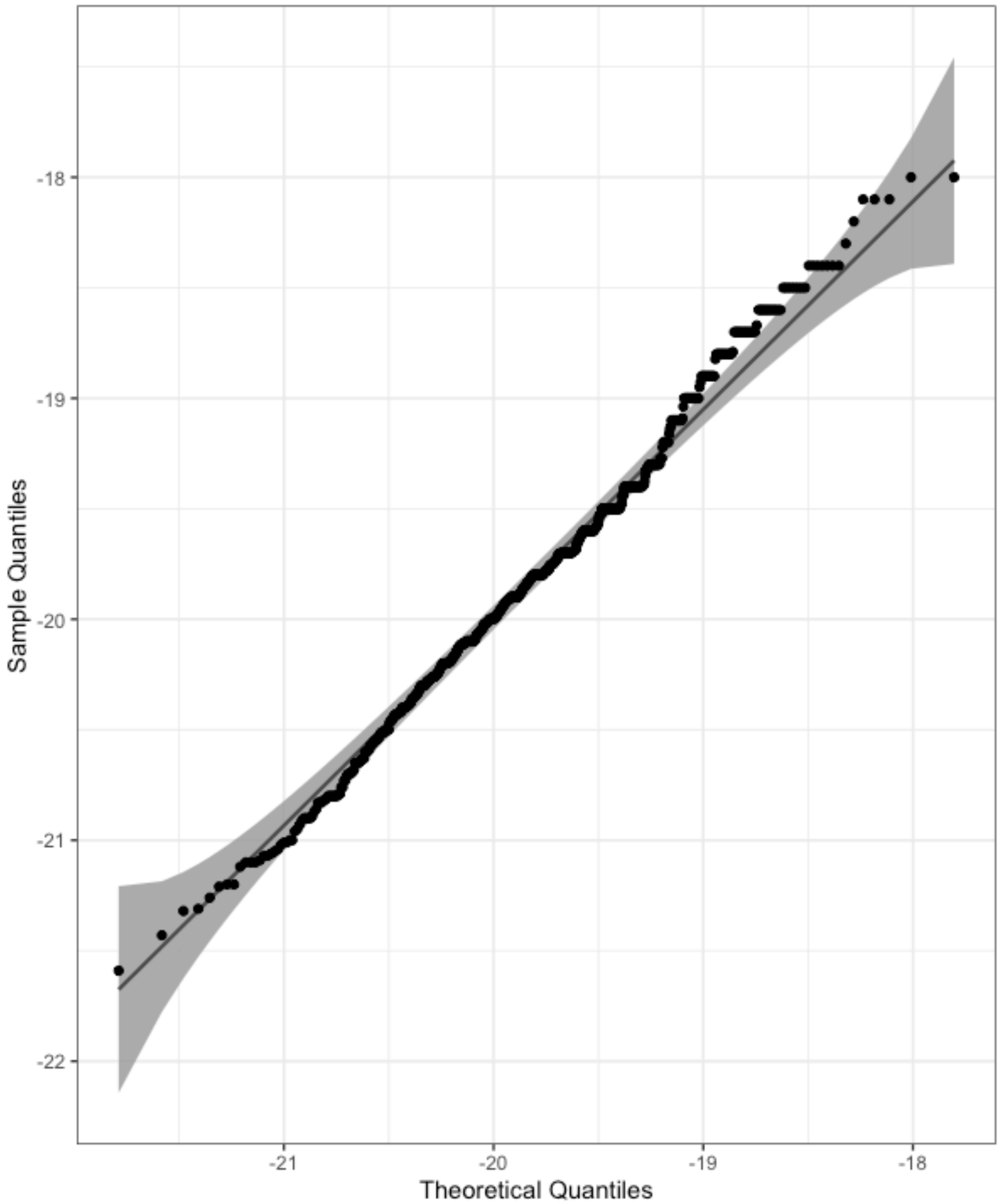


Figure C-9: q-q plot for dentine δ¹³C values in the whole human England dataset.

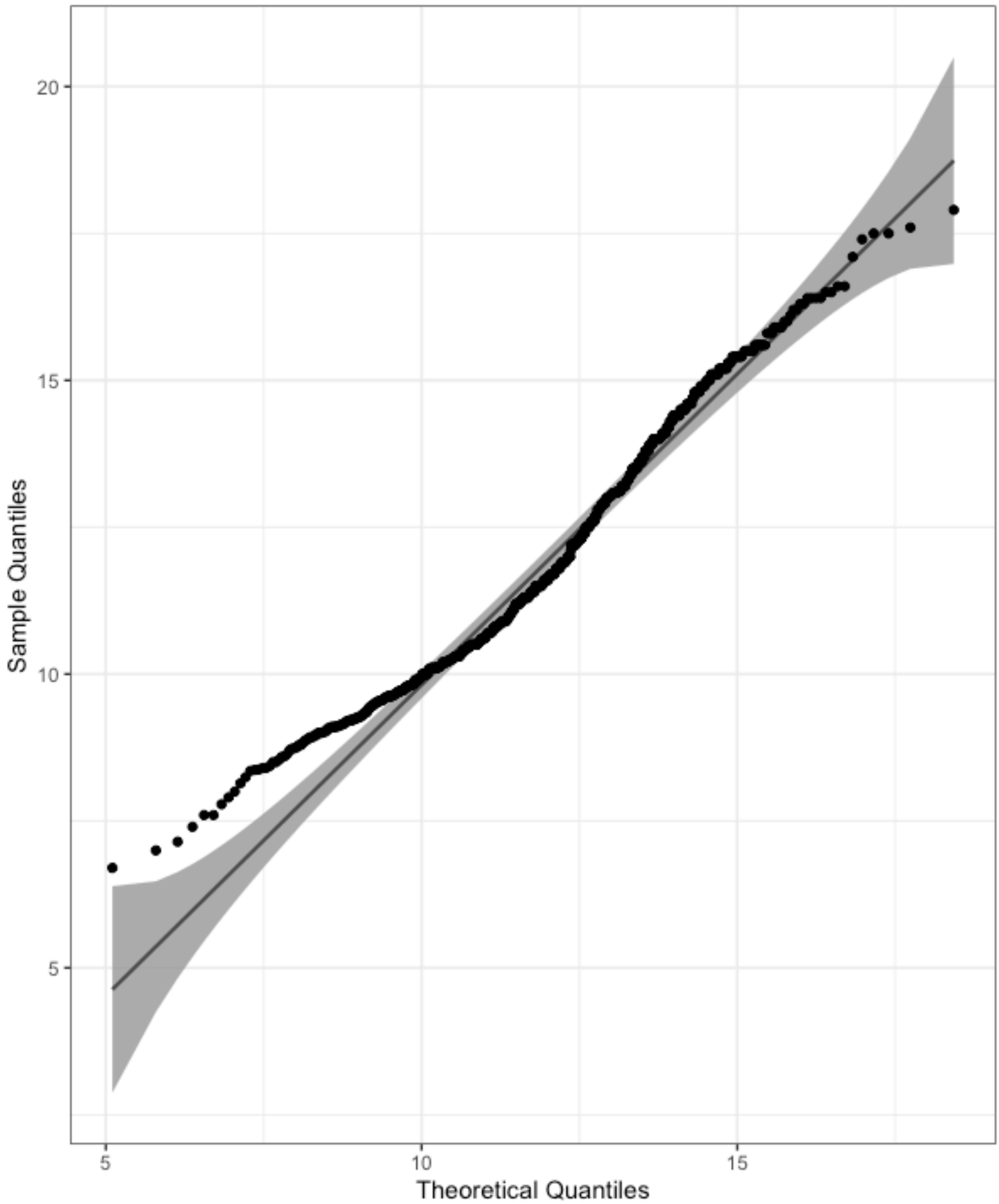


Figure C-10: q-q plot for dentine $\delta^{15}N$ values in the whole human England dataset.

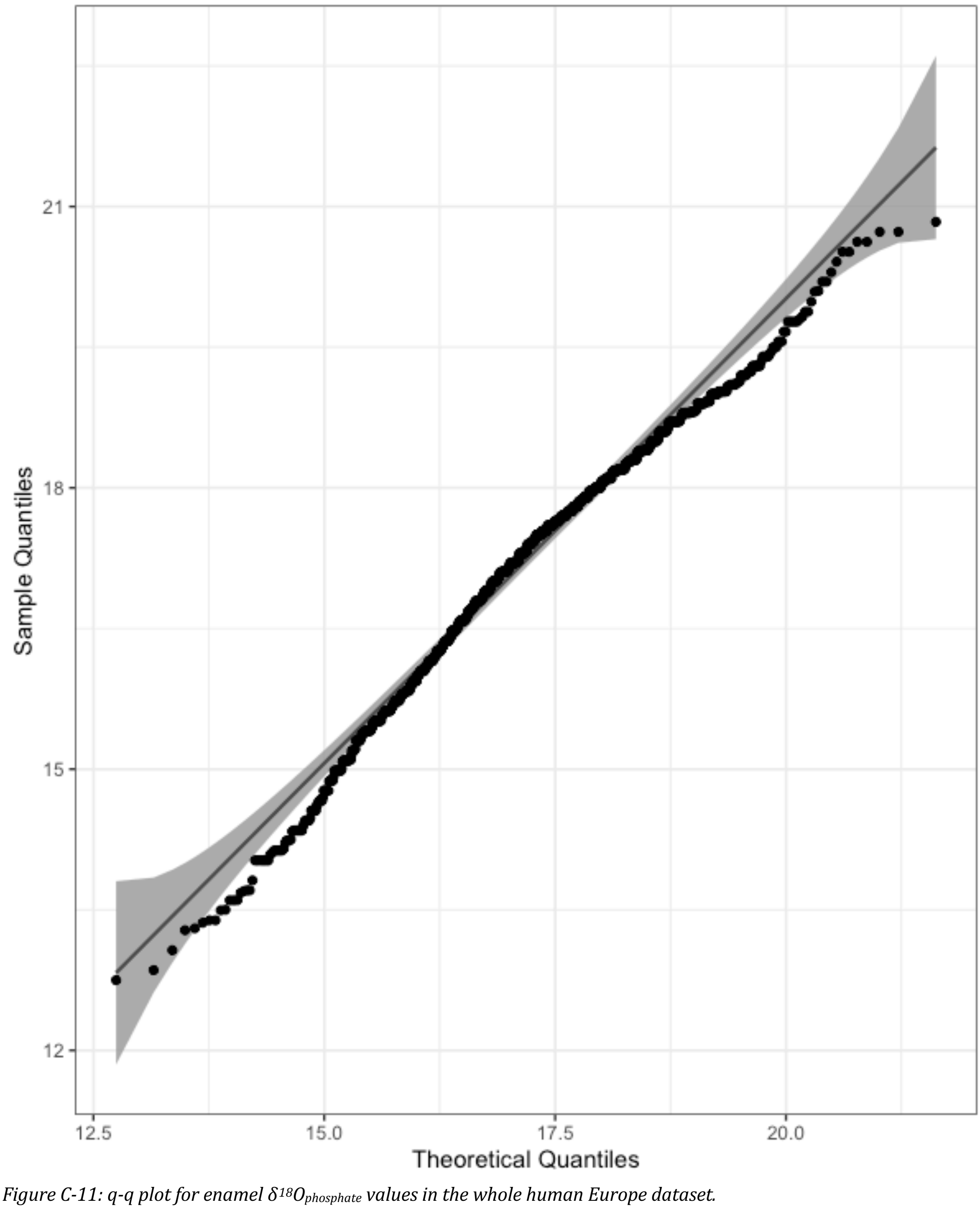


Figure C-11: q-q plot for enamel $\delta^{18}O_{phosphate}$ values in the whole human Europe dataset.

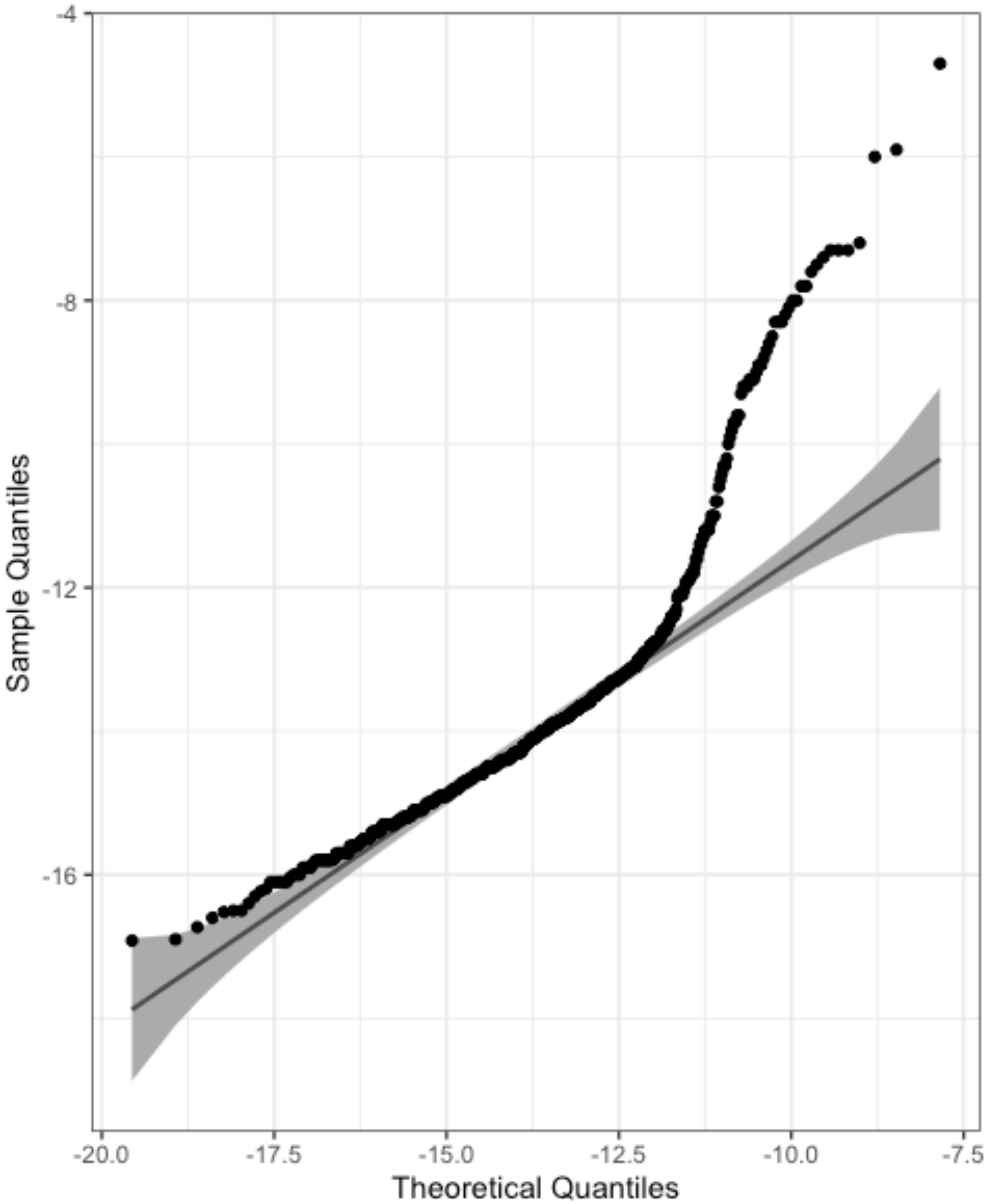


Figure C-12: q-q plot for enamel $\delta^{13}C_{carb}$ values in the whole human Europe dataset.

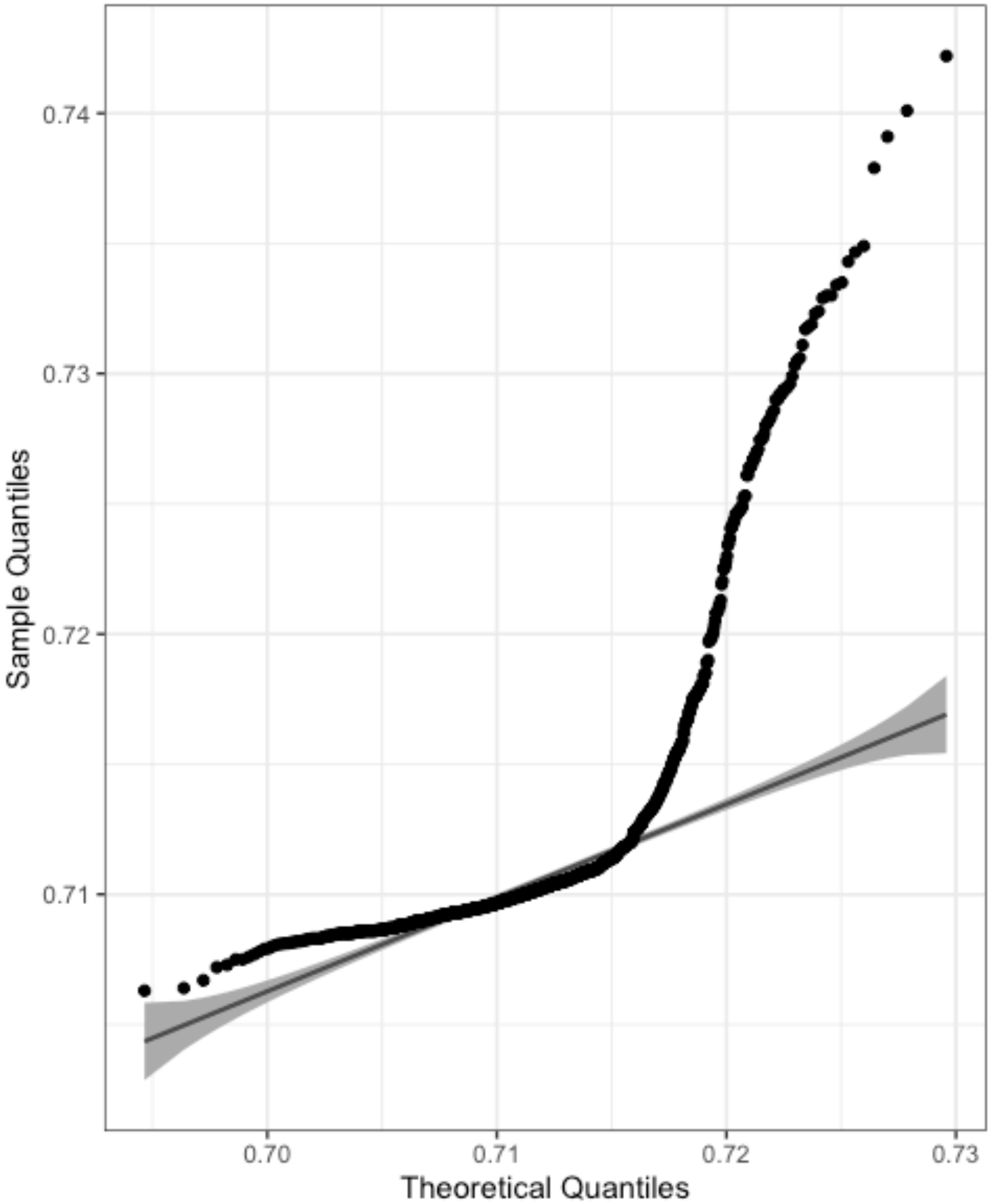


Figure C-13: q-q plot for enamel $^{87/86}Sr$ values in the whole human Europe dataset.

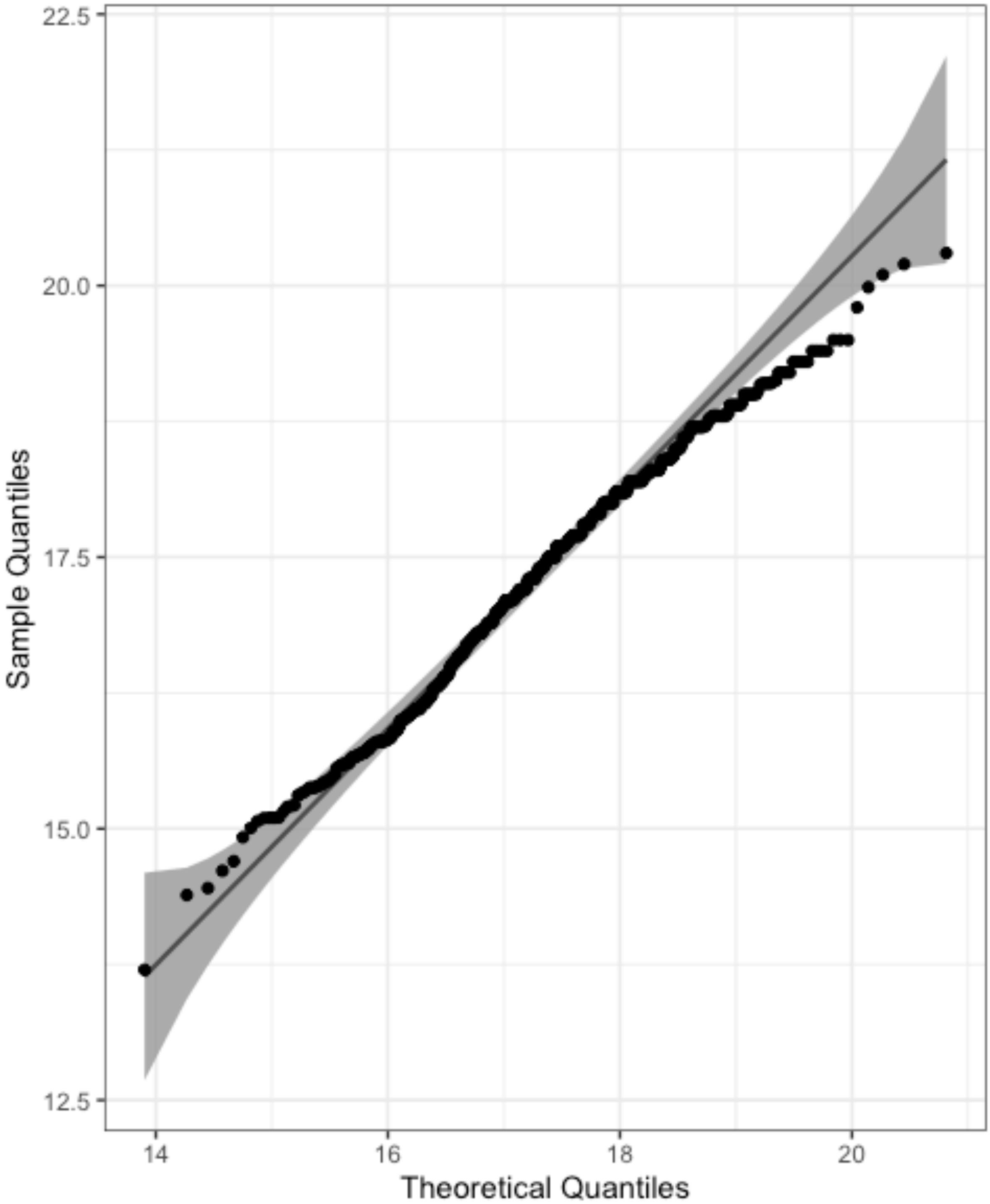


Figure C-14: q-q plot for enamel $\delta^{18}O_{phosphate}$ values in the whole human England dataset.

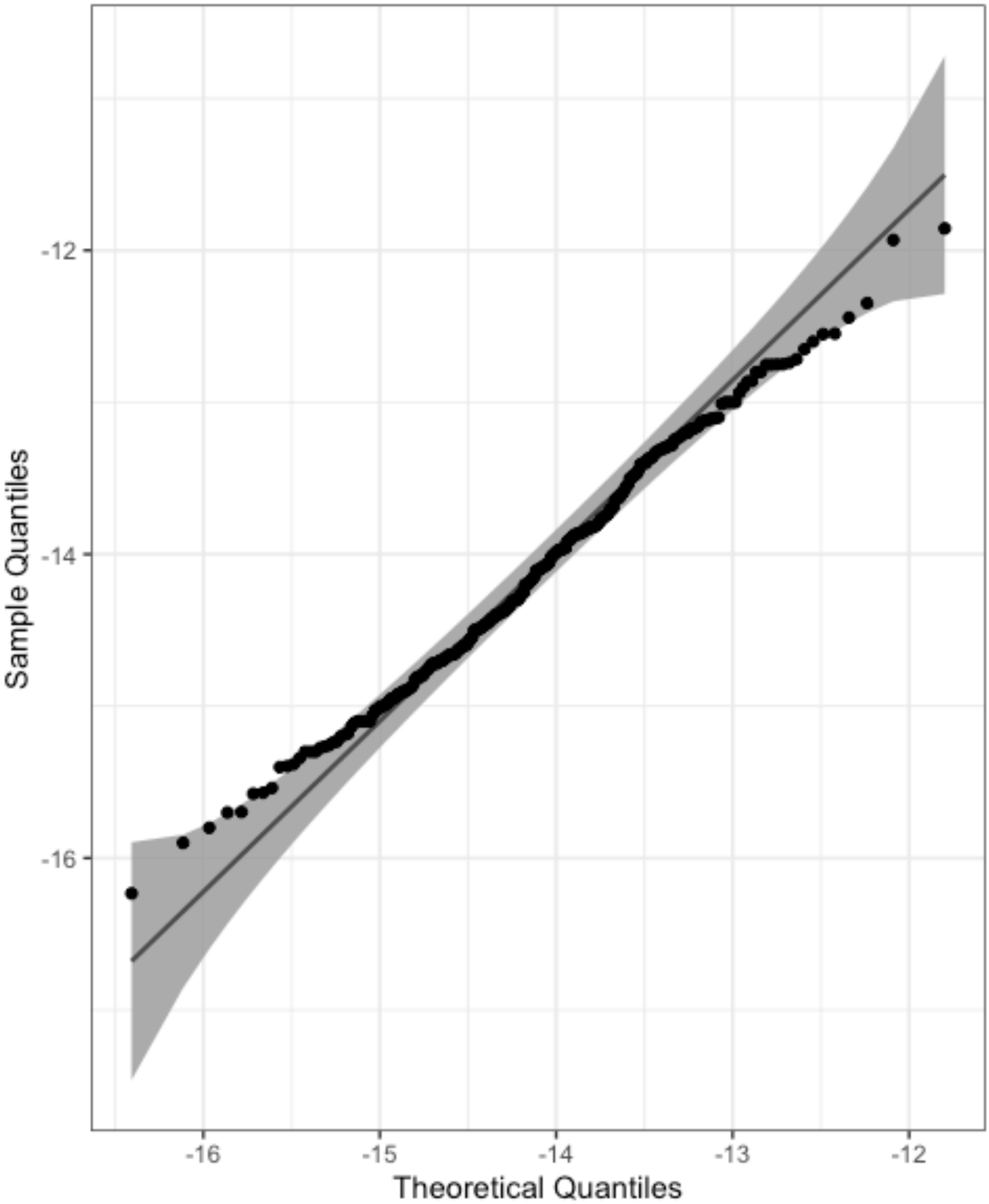


Figure C-15: q-q plot for enamel $\delta^{13}C_{carb}$ values in the whole human England dataset.

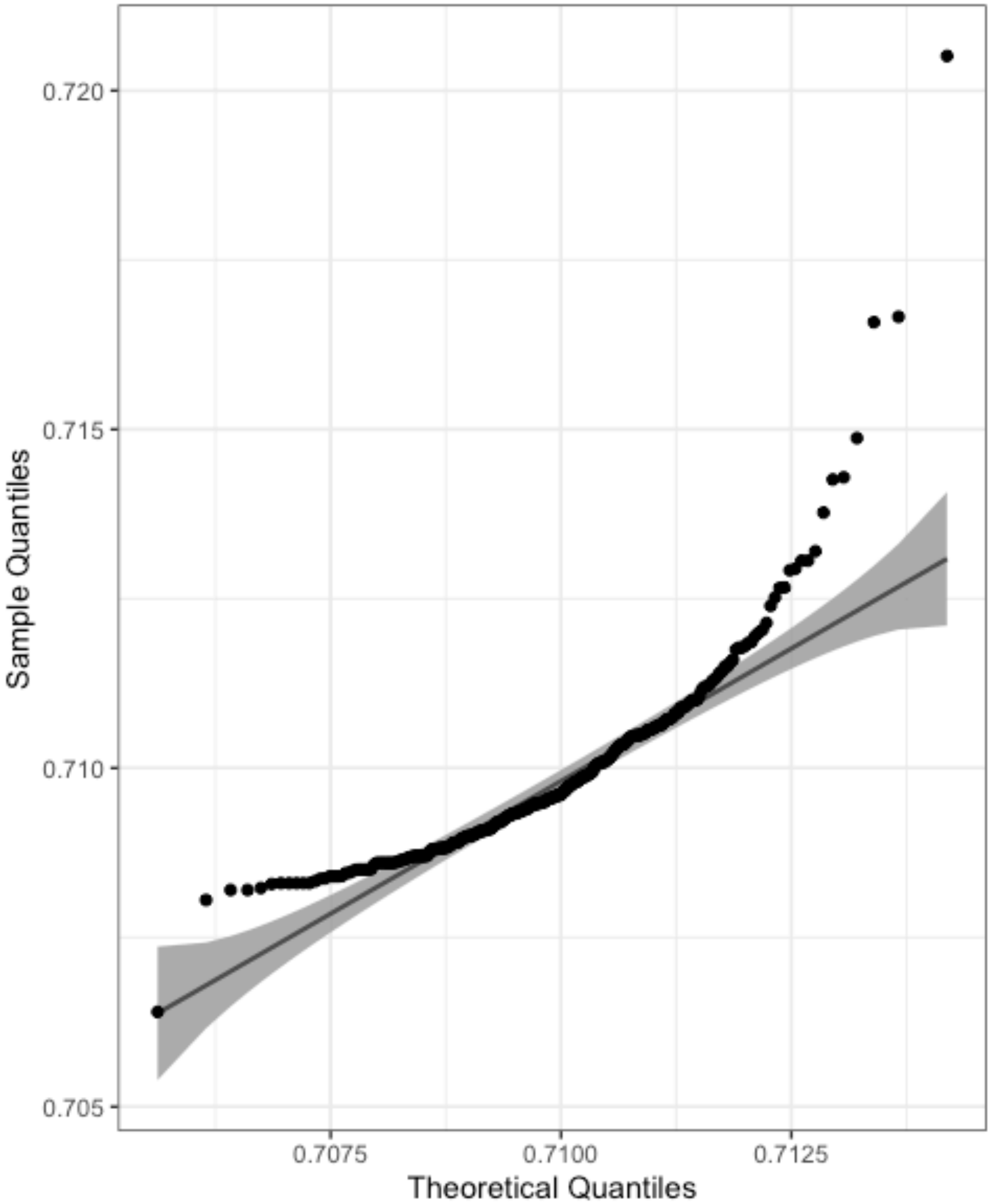


Figure C-16: q-q plot for enamel $^{87/86}Sr$ values in the whole human England dataset.

D BEST Test Outputs

D.i Outputs for Geology in England

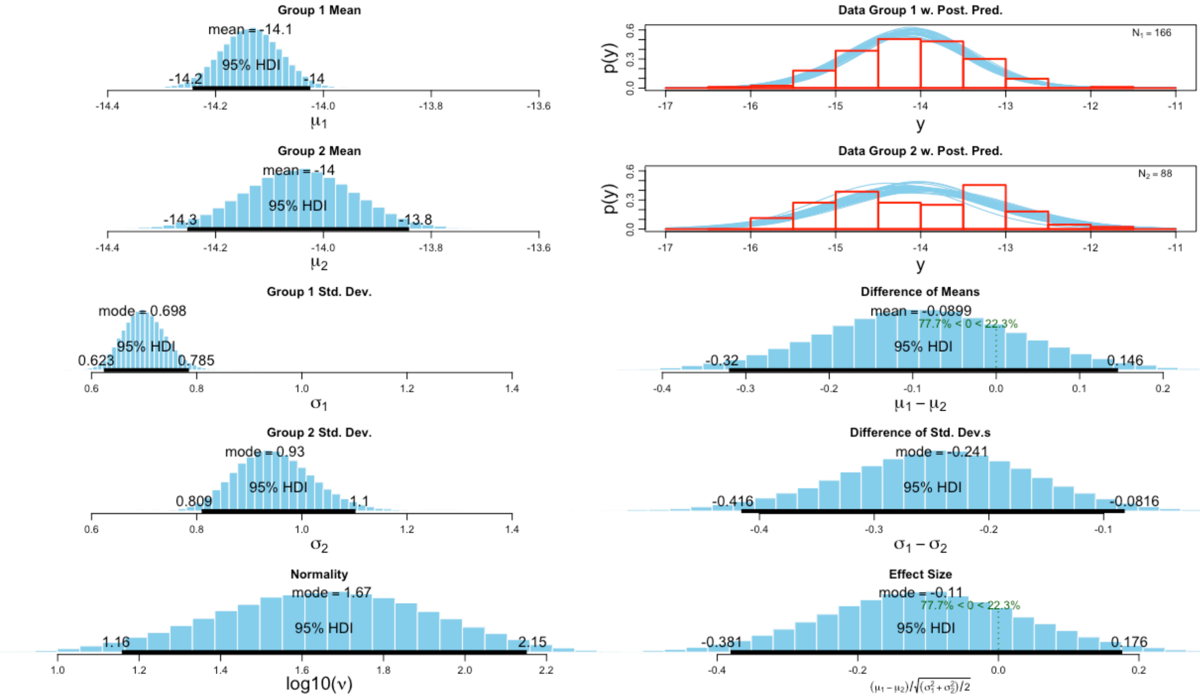


Figure D-1: BEST test output for chalk (group 1) vs other geologies (group 2) enamel δ13C values for England.

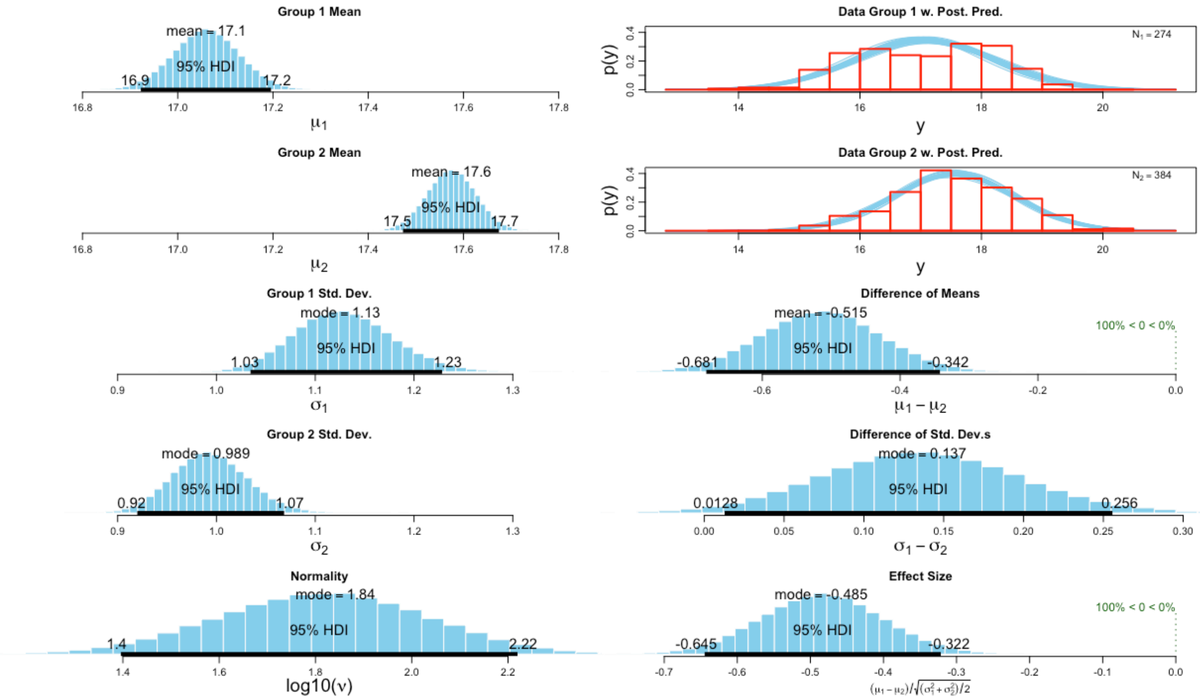


Figure D-2: BEST test output for chalk (group 1) vs other geologies (group 2) enamel δ18O values for England.

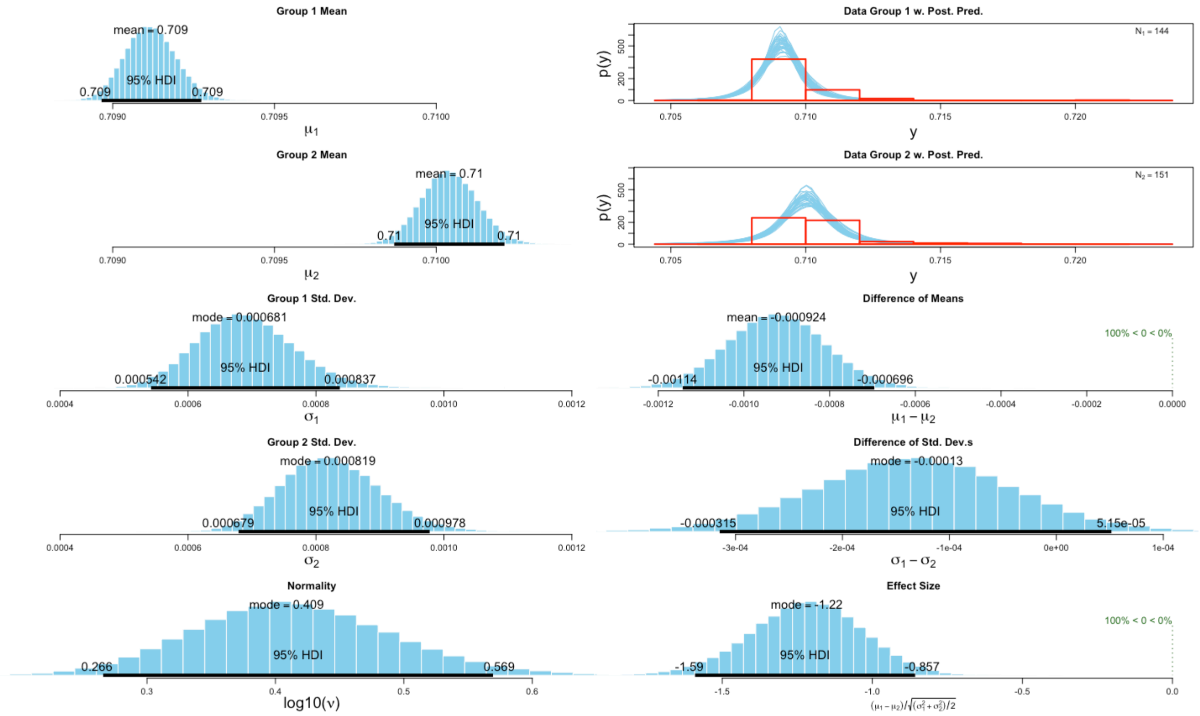


Figure D-3: BEST test output for chalk (group 1) vs other geologies (group 2) enamel $^{87/86}$Sr values for England.

D.ii Outputs for Female vs. Male δ18O values

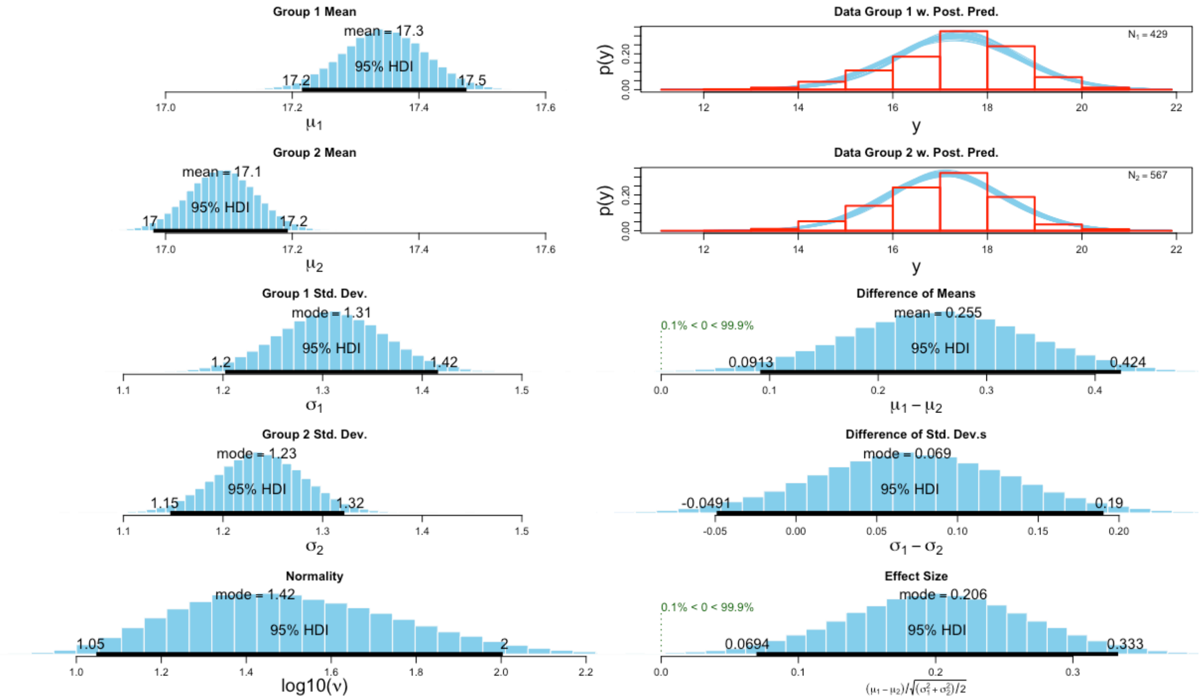


Figure D-4: BEST test output for females (group 1) vs males (group 2) $\delta^{18}O$ values for the whole of Europe.

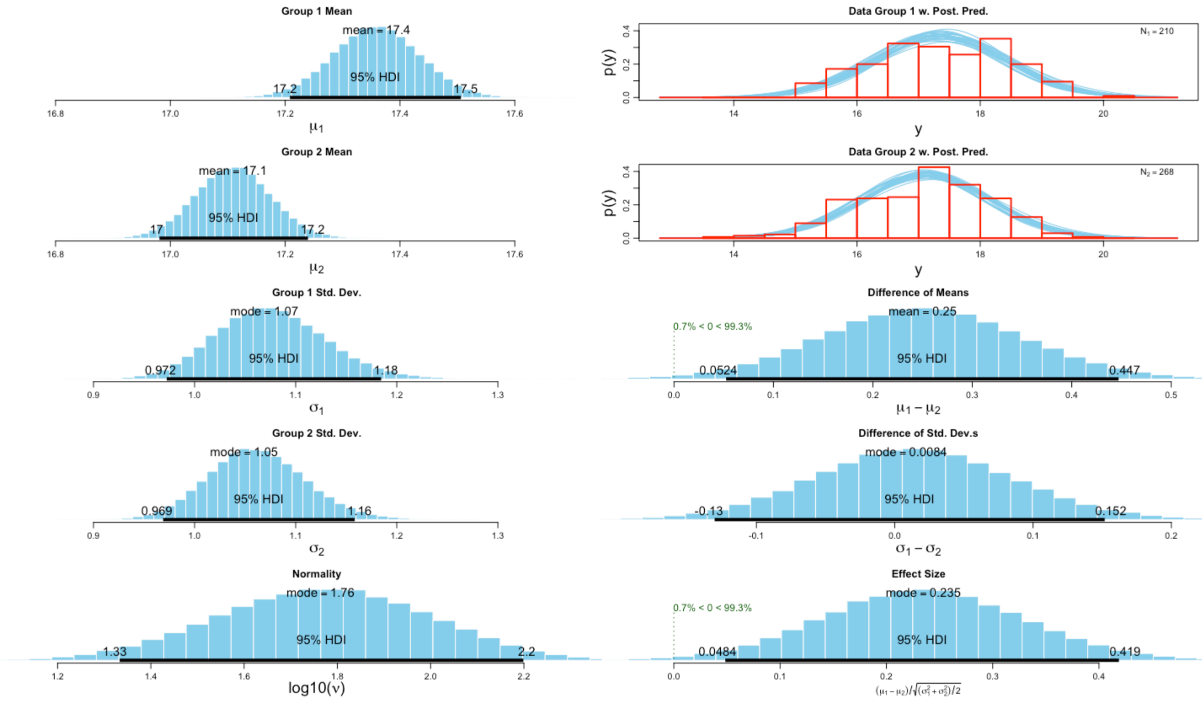


Figure D-5: BEST test output for females (group 1) vs males (group 2) δ18O values for England across all time periods.

D.ii.i Outputs for Female vs. Male δ18O values through time

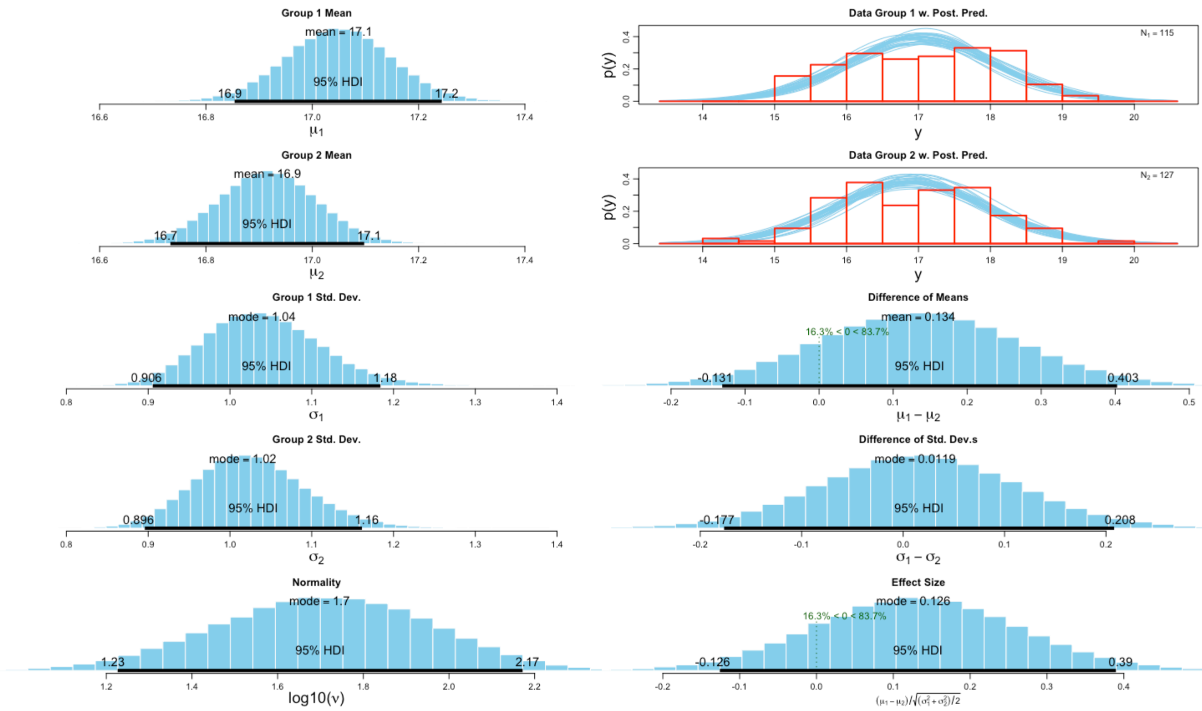


Figure D-6: BEST test output for females (group 1) vs males (group 2) δ18O values for England for the period c. 350-790 AD.

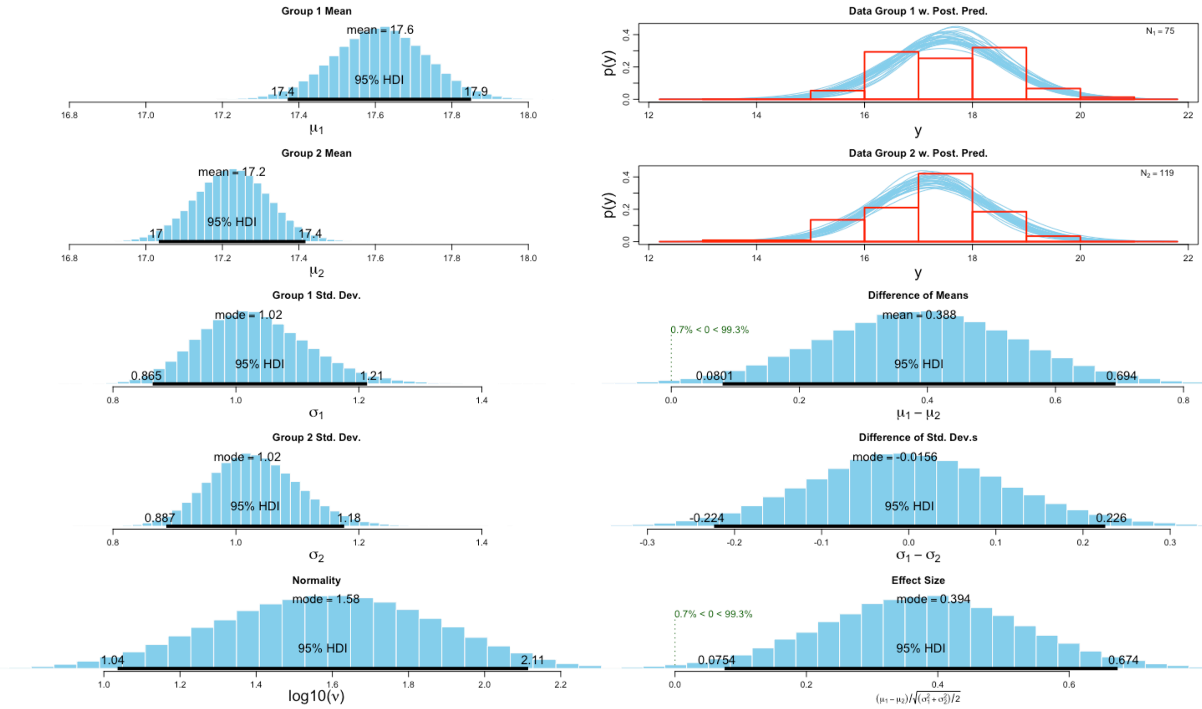


Figure D-7: BEST test output for females (group 1) vs males (group 2) δ18O values for England for the period c. 790-1200 AD.

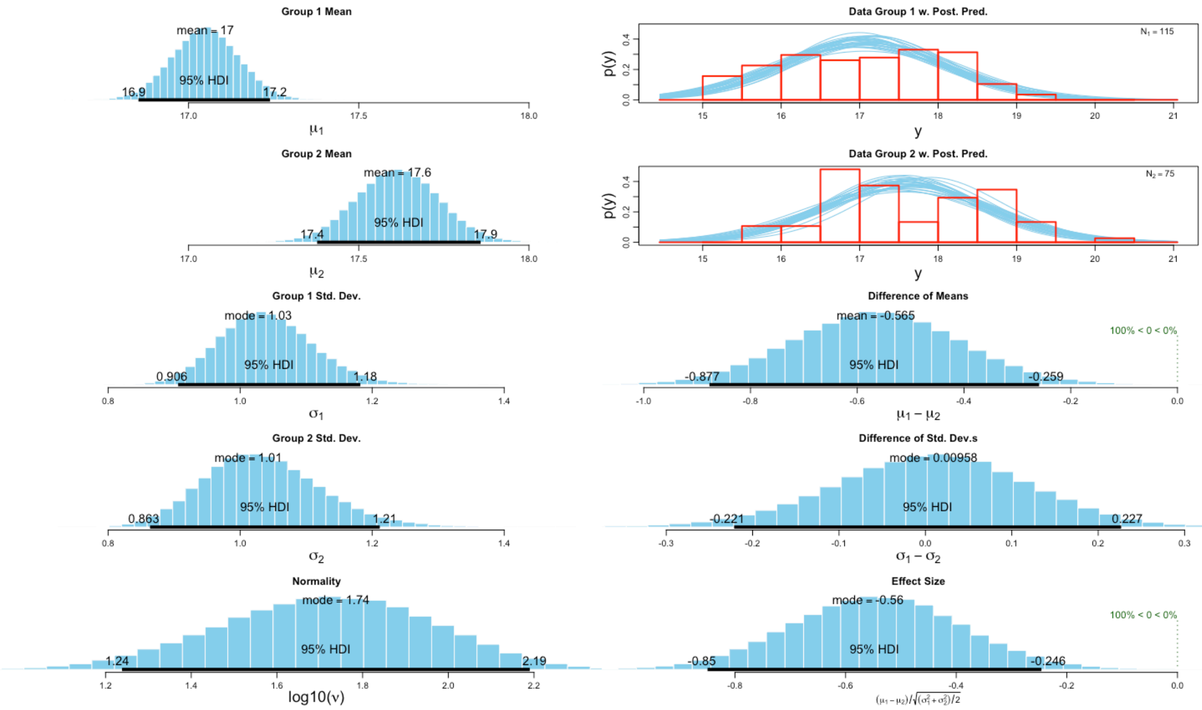


Figure D-8: BEST test output for females c. 350-790 AD(group 1) vs females c.790-1200 AD (group 2) δ18O values for England.

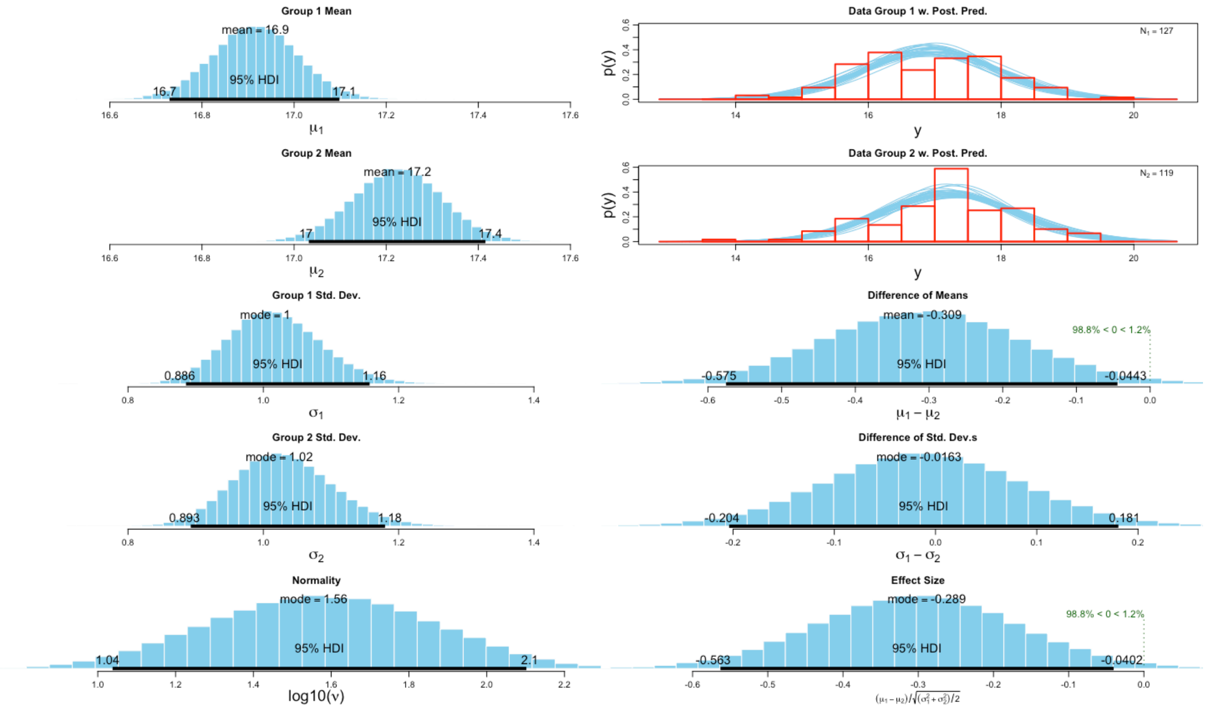


Figure D-9: BEST test output for males c. 350-790 AD(group 1) vs males c.790-1200 AD (group 2) $\delta^{18}O$ values for England.

D.iii Outputs through time

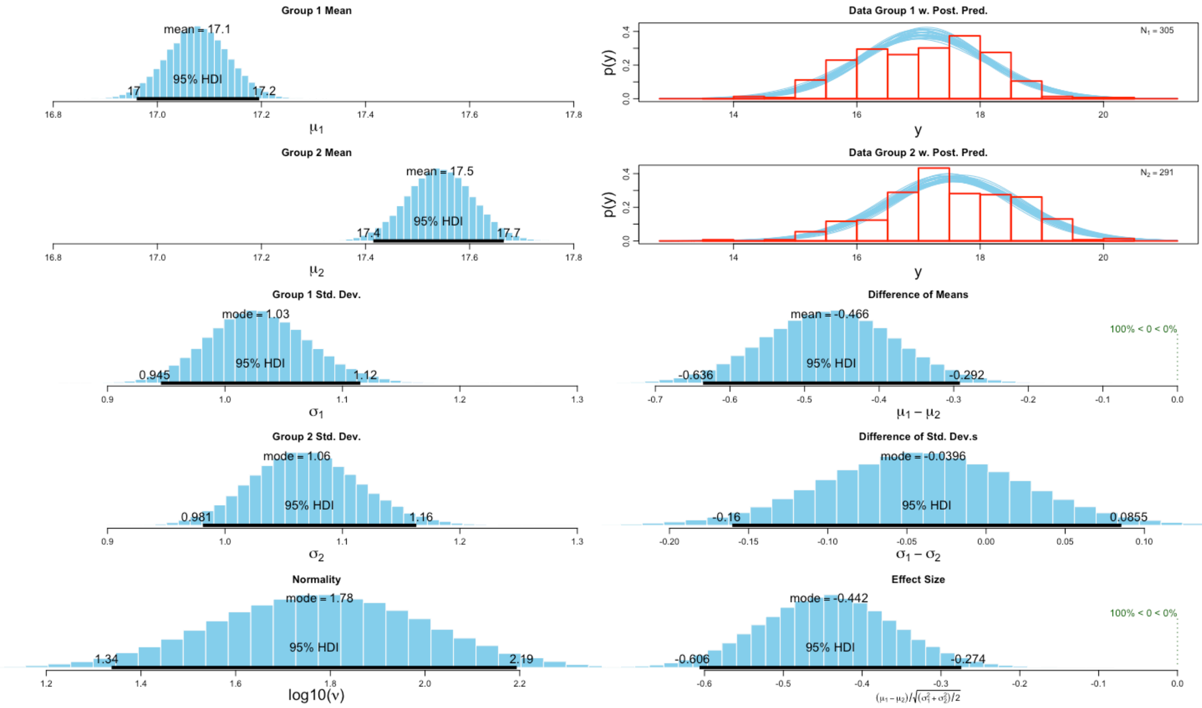


Figure D-10: BEST test output for c. 350-790 AD(group 1) vs c.790-1200 AD (group 2) $\delta^{18}O$ values for England (all sexes).

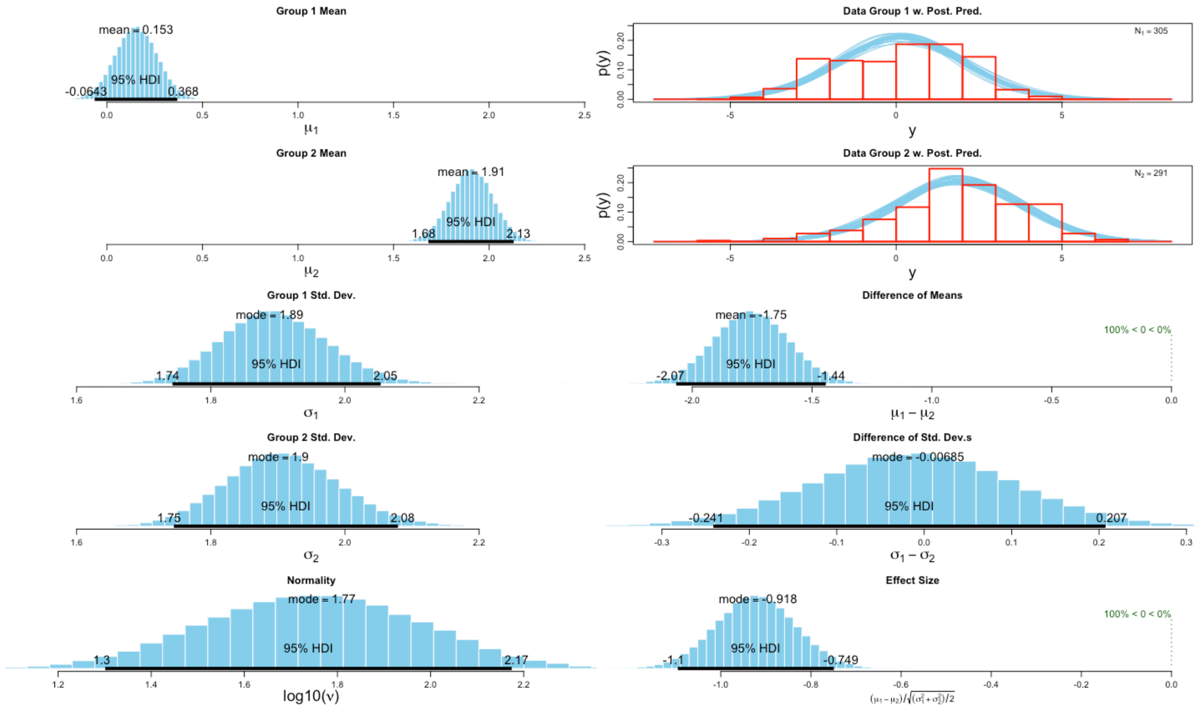


Figure D-11: BEST test output for c. 350-790 AD(group 1) vs c.790-1200 AD (group 2) $\Delta^{18}O_{dw\text{-}MAP\ (Chenery)}$ values for England (all sexes).

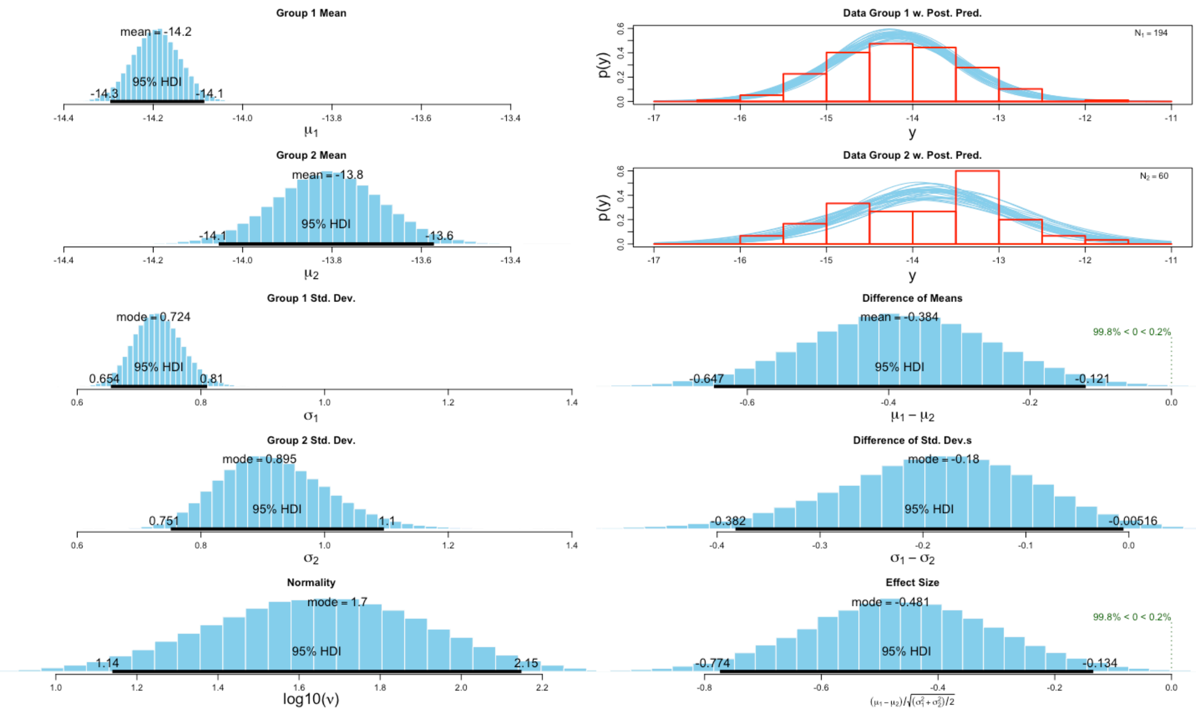


Figure D-12: BEST test output for c. 350-790 AD(group 1) vs c.790-1200 AD (group 2) enamel $\delta^{13}C_{carb}$ values for England (all sexes).

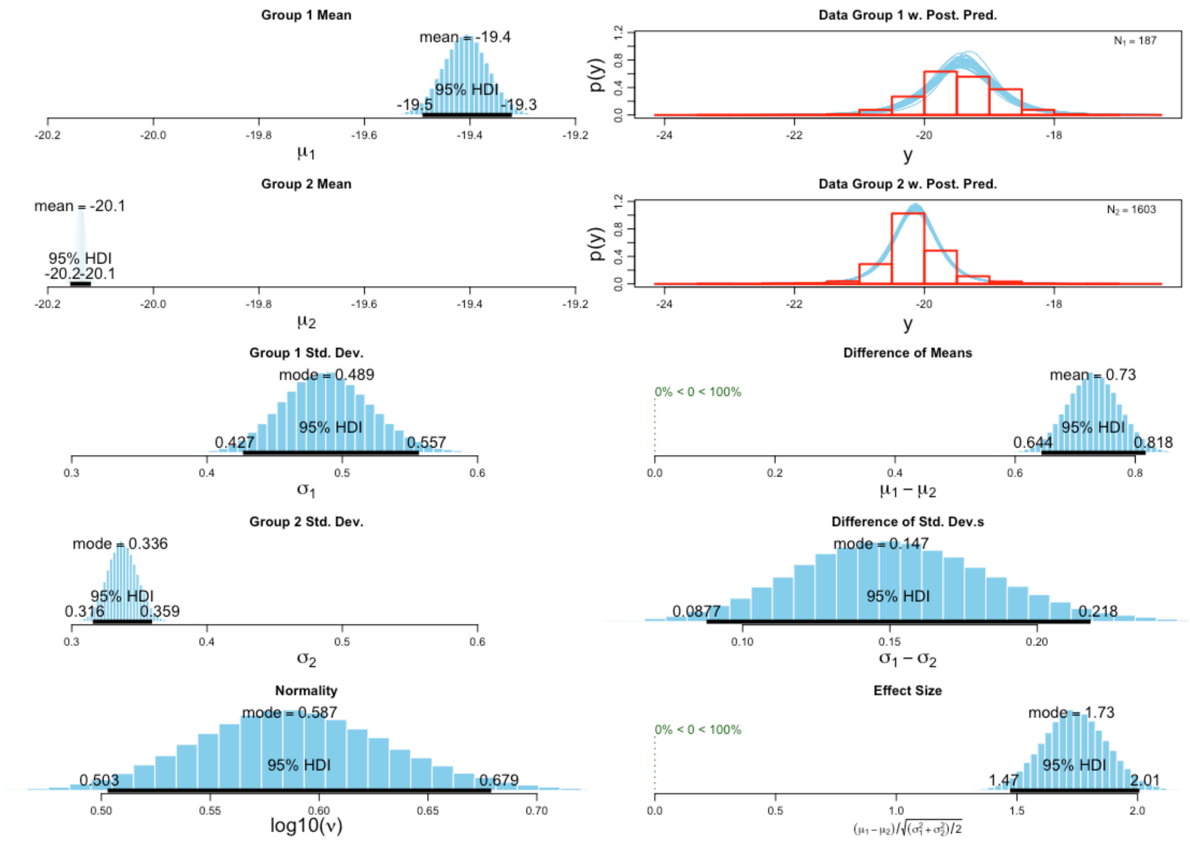


Figure D-13: BEST test output for c. 200BC – 450 AD (group 1) vs c. 400-790 AD (group 2) bone δ13Ccoll values for England (all sexes).

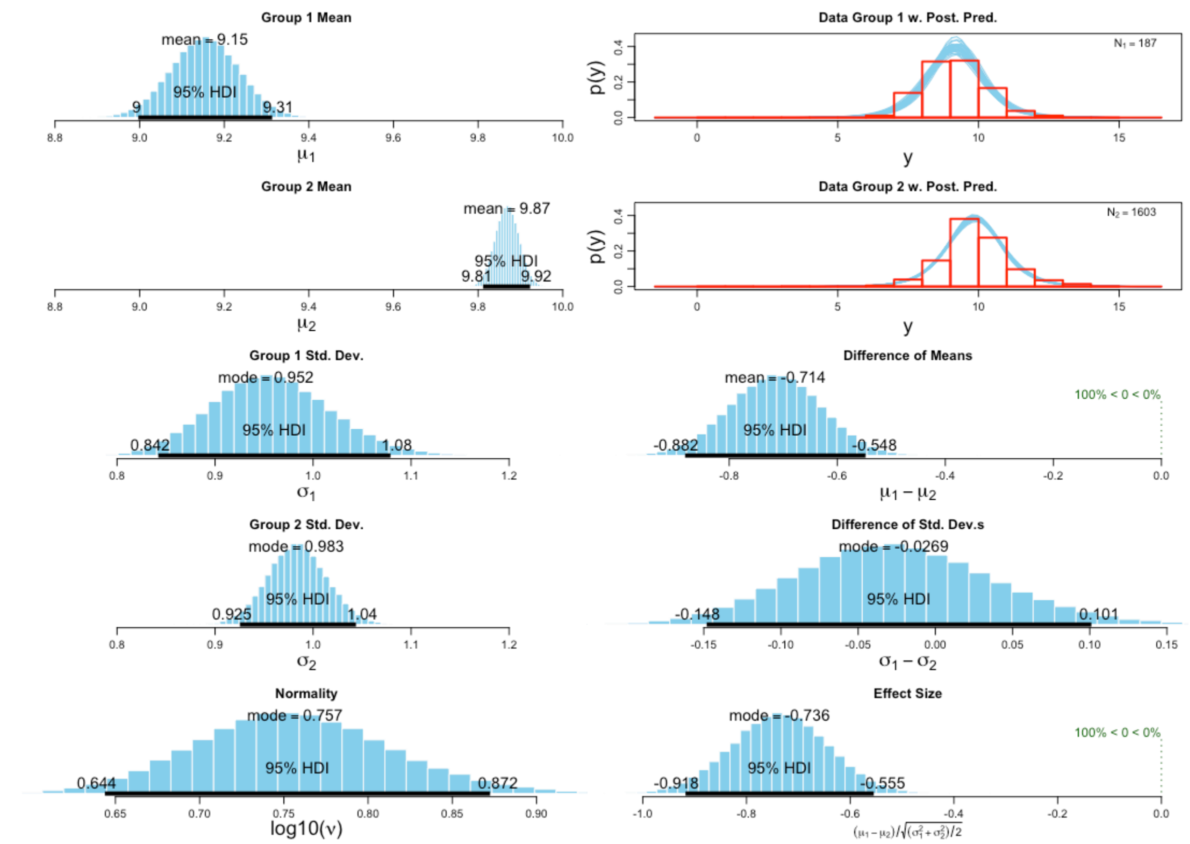


Figure D-14: BEST test output for c. 200BC – 450 AD (group 1) vs c. 400-790 AD (group 2) bone δ15Ncoll values for England (all sexes).

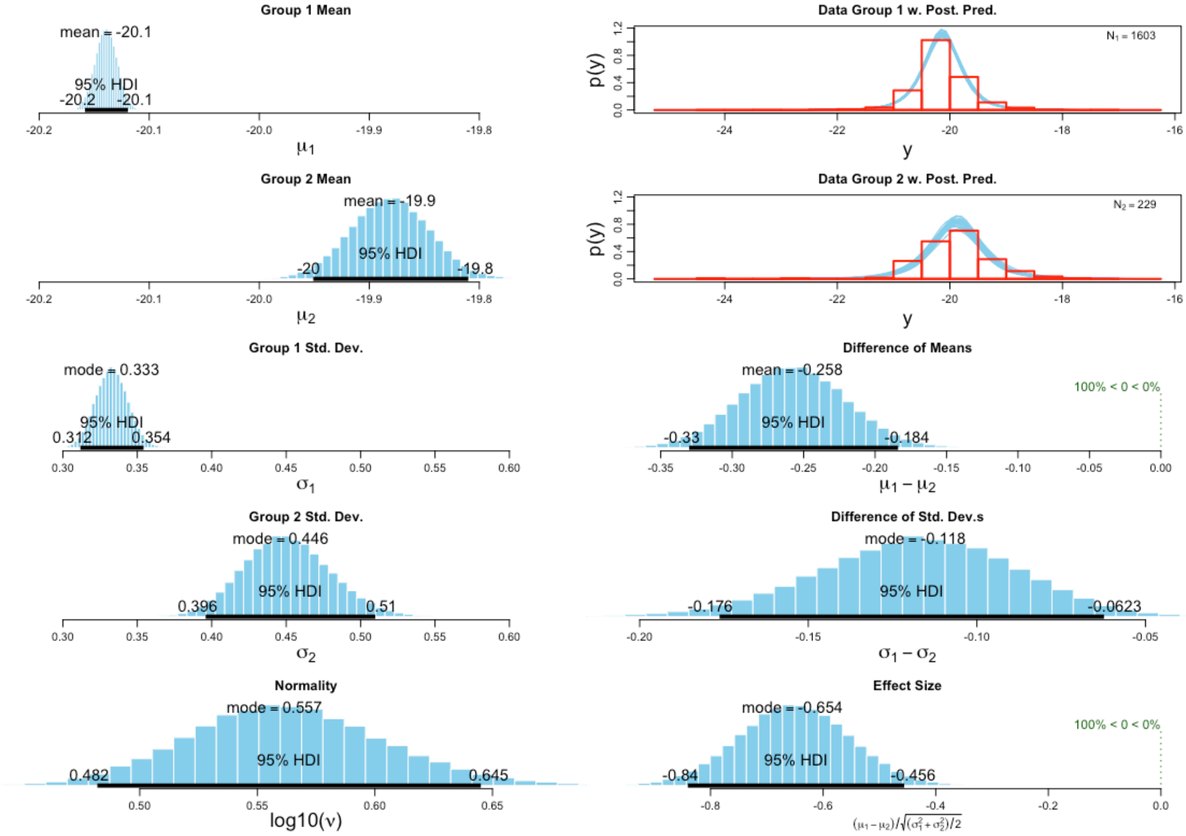


Figure D-15: BEST test output for c. 350-790 AD (group 1) vs c.790-1200 AD (group 2) bone $\delta^{13}C_{coll}$ values for England (all sexes).

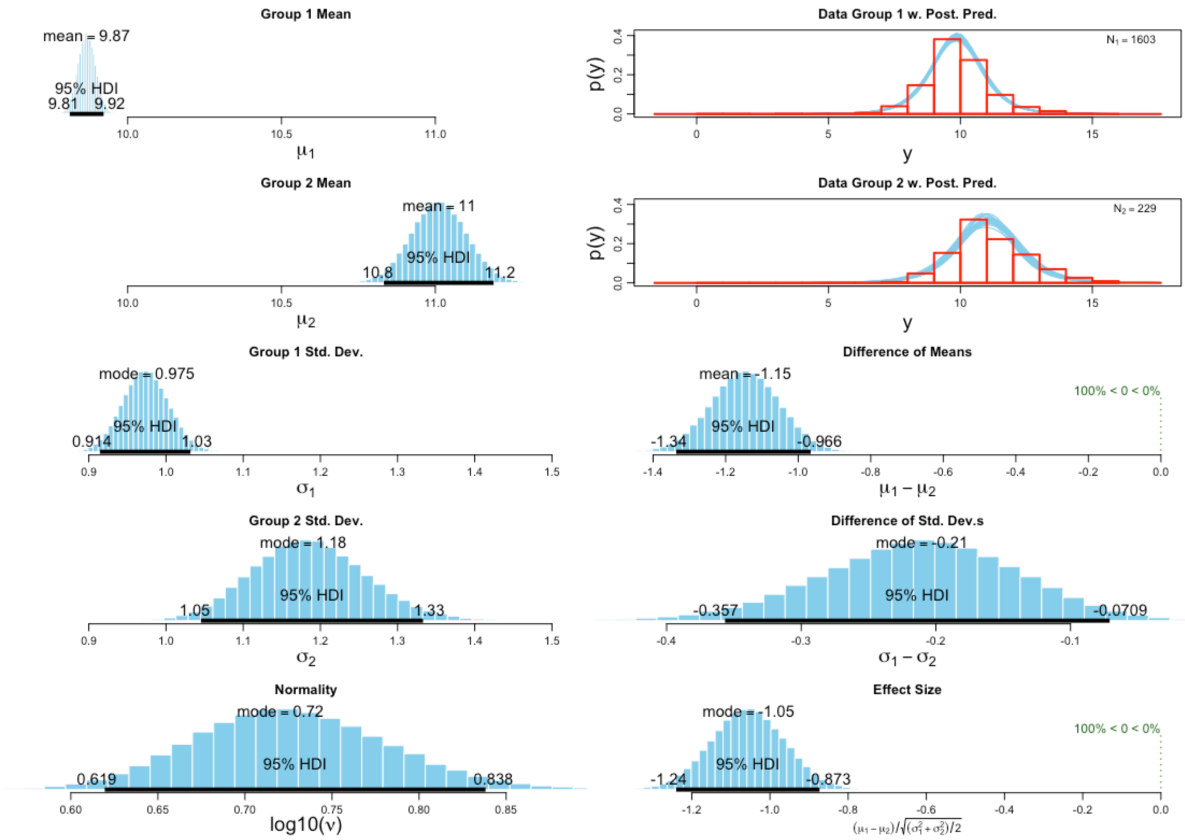


Figure D-16: BEST test output for c. 350-790 AD (group 1) vs c.790-1200 AD (group 2) bone $\delta^{15}N_{coll}$ values for England (all sexes).

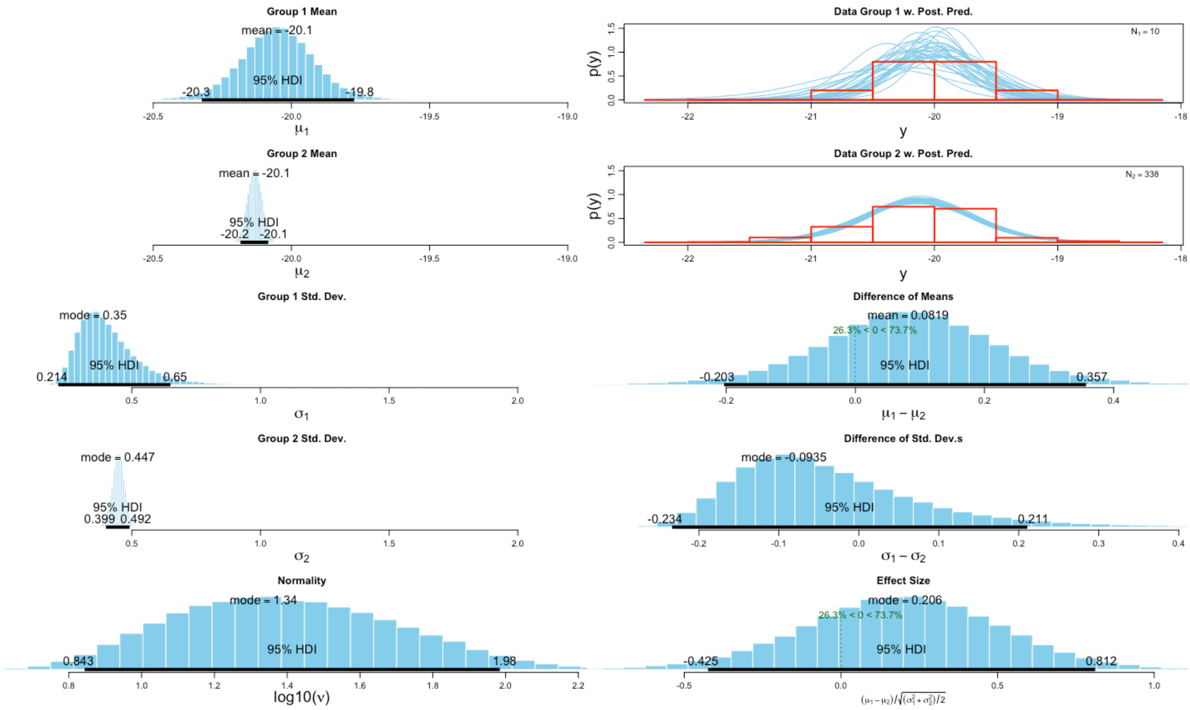


Figure D-17: BEST test output for c. 200BC – 450 AD (group 1) vs c. 400-790 AD (group 2) dentine δ¹³C$_{coll}$ values for England (all sexes).

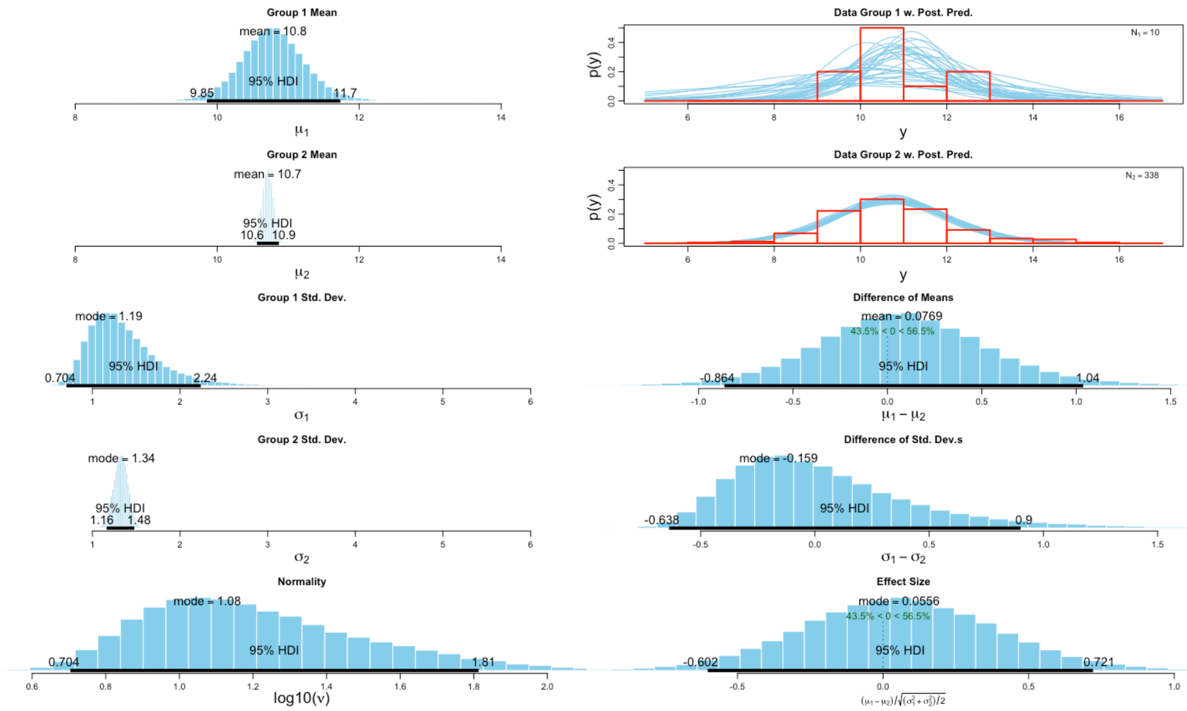


Figure D-18: BEST test output for c. 200BC – 450 AD (group 1) vs c. 400-790 AD (group 2) dentine δ¹⁵N$_{coll}$ values for England (all sexes).

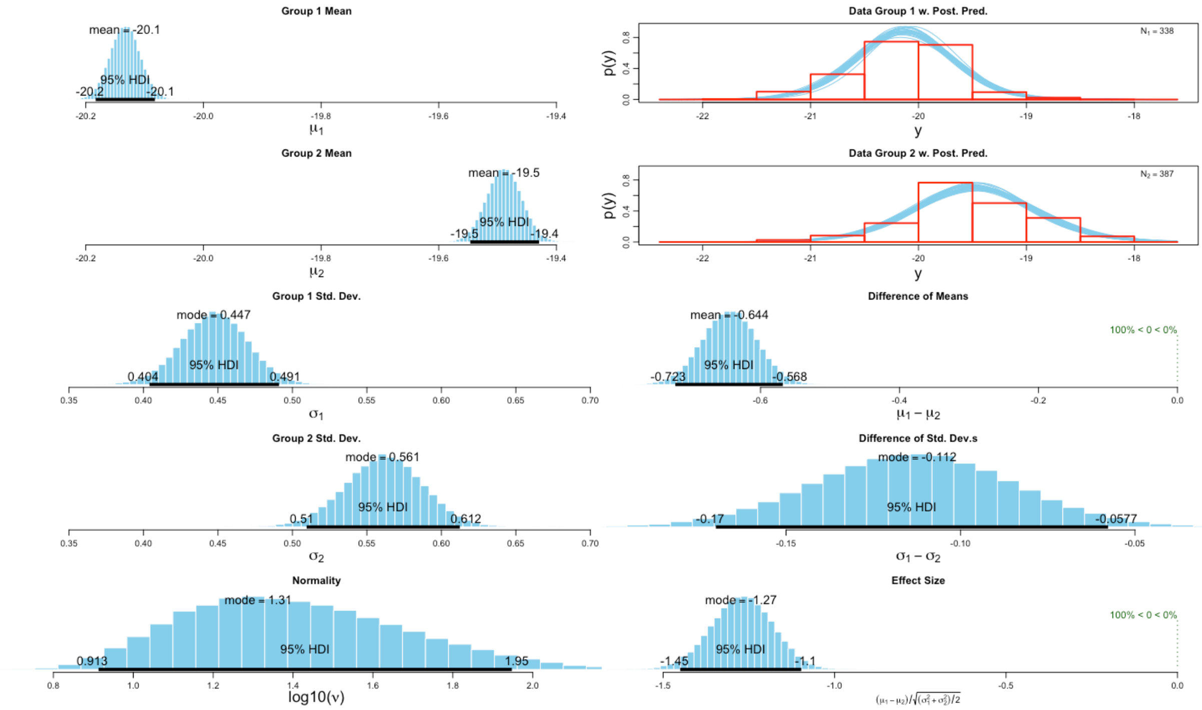


Figure D-19: BEST test output for c. 350-790 AD(group 1) vs c.790-1200 AD (group 2) dentine δ¹³C$_{coll}$ values for England (all sexes).

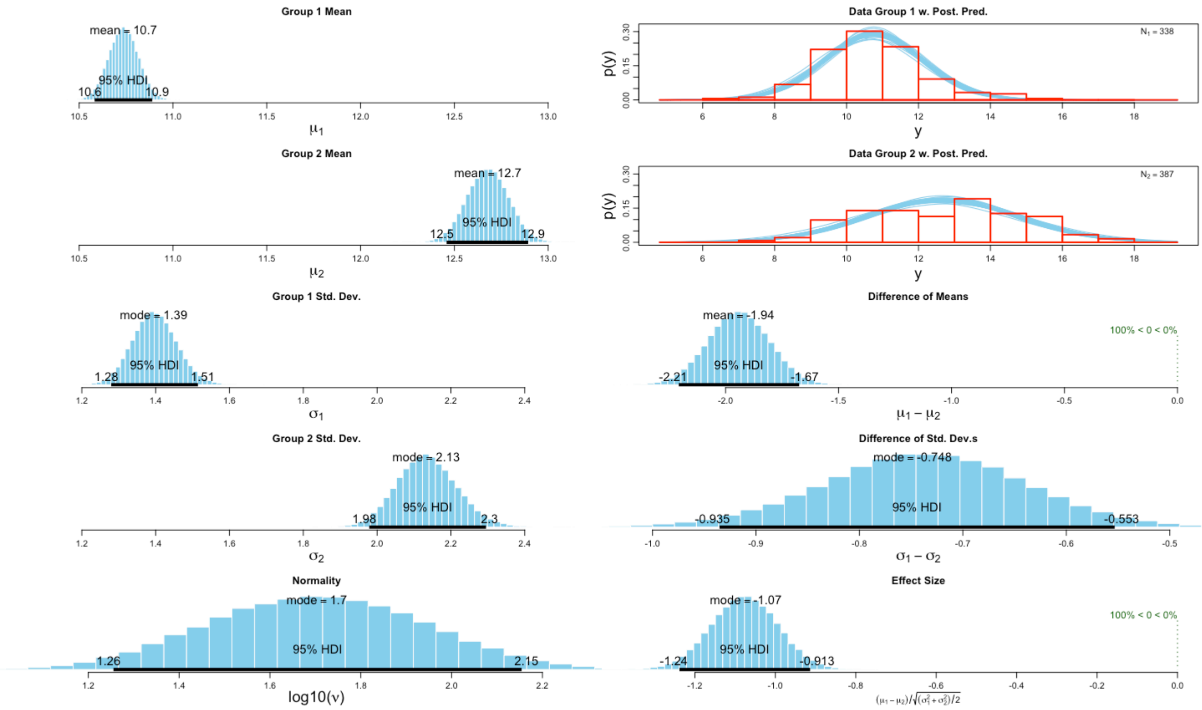


Figure D-20: D-21: BEST test output for c. 350-790 AD (group 1) vs c.790-1200 AD (group 2) dentine δ¹⁵N$_{coll}$ values for England (all sexes).

D.iv Outputs for enamel $\delta^{13}C$, bone and dentine in England by sex

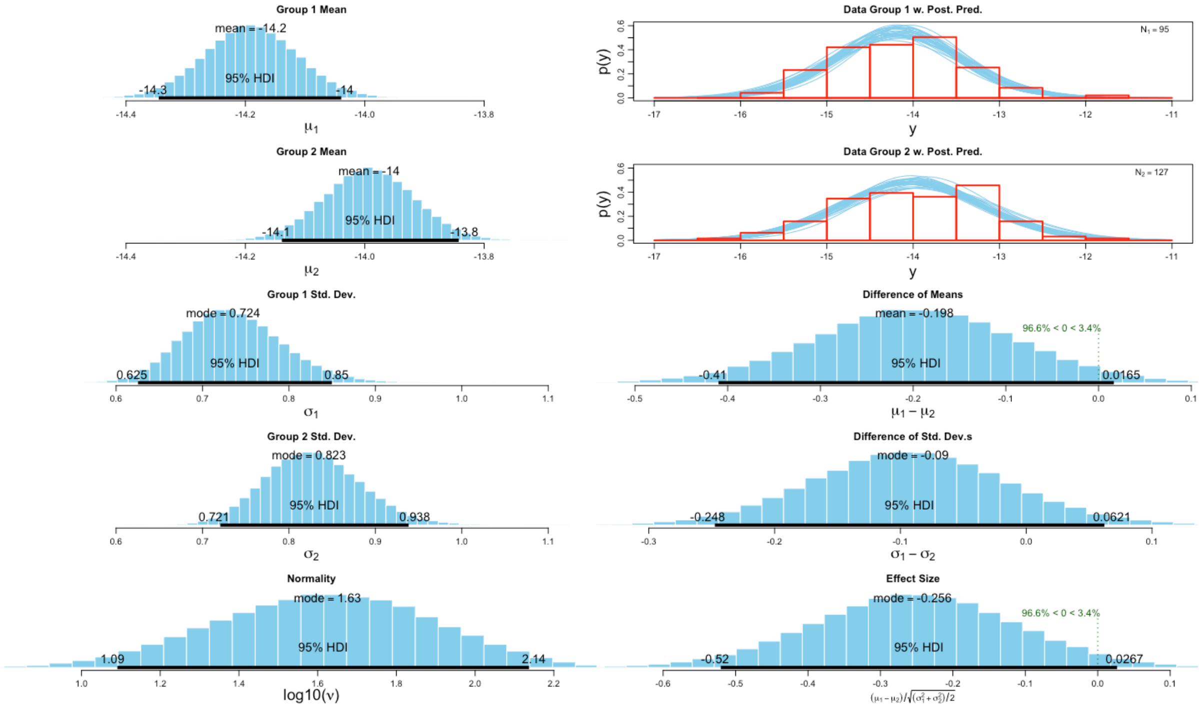


Figure D-22: BEST test output for females (group 1) vs males (group 2) enamel $\delta^{13}C_{carb}$ values in England.

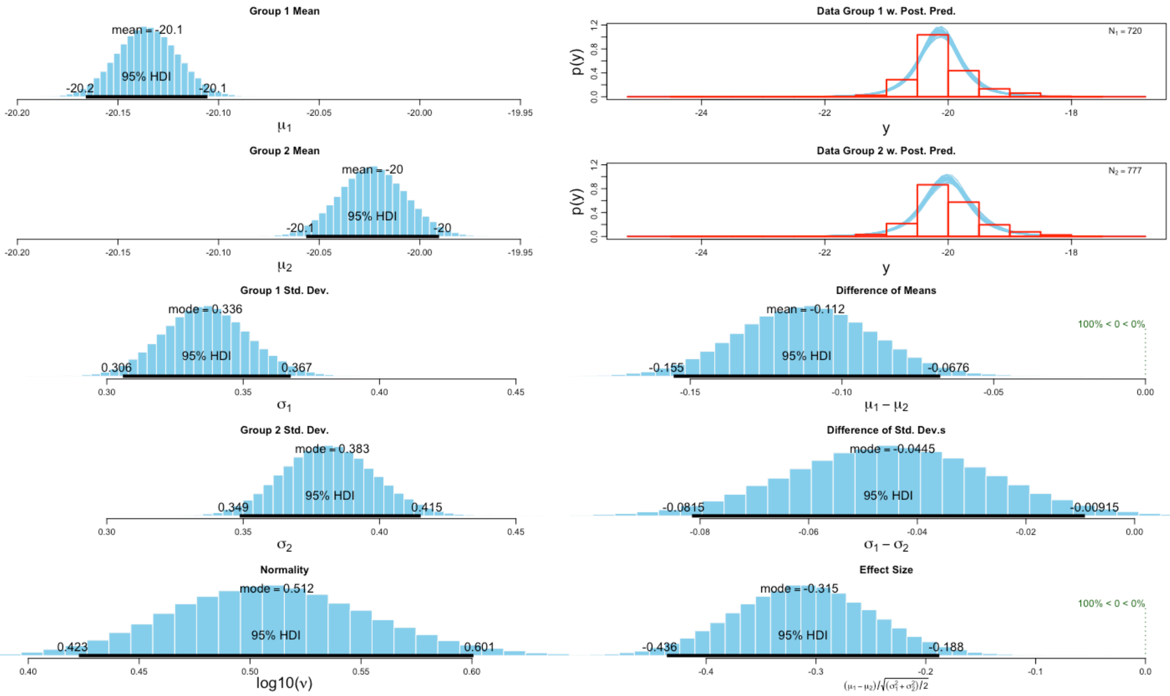


Figure D-23: BEST test output for females (group 1) vs males (group 2) bone $\delta^{13}C_{coll}$ values in England.

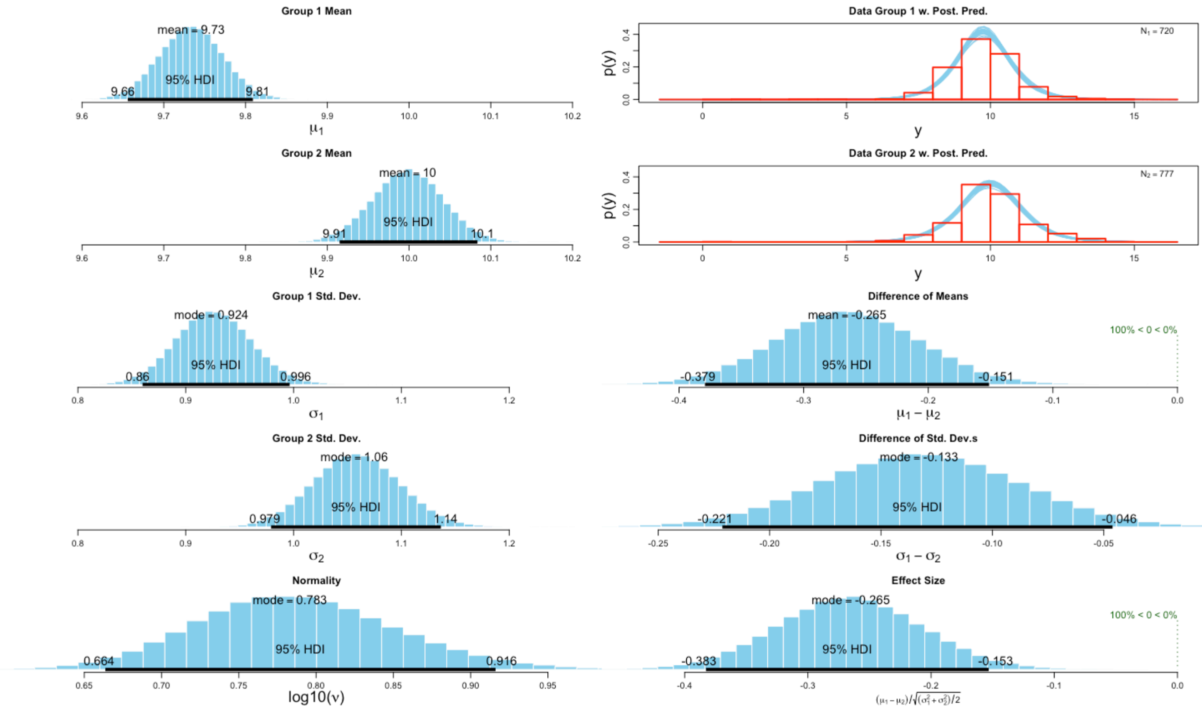


Figure D-24: BEST test output for females (group 1) vs males (group 2) bone $\delta^{15}N_{coll}$ values in England.

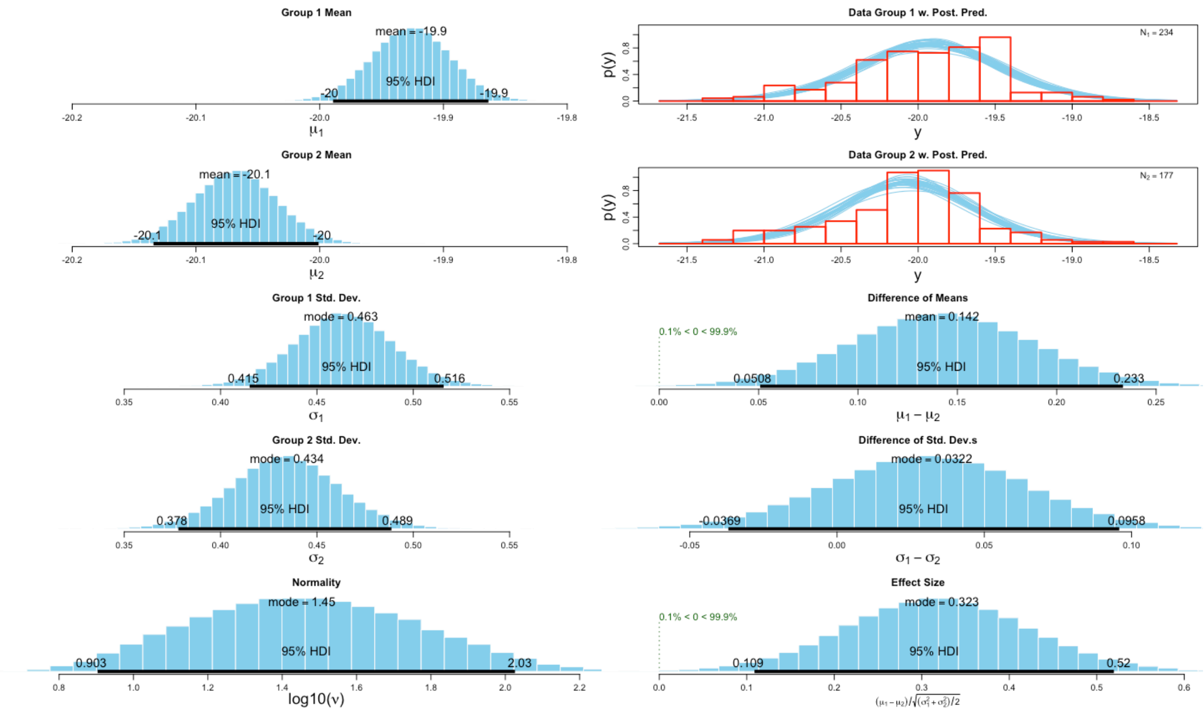


Figure D-25: BEST test output for females (group 1) vs males (group 2) dentine $\delta^{13}C_{coll}$ values in England.

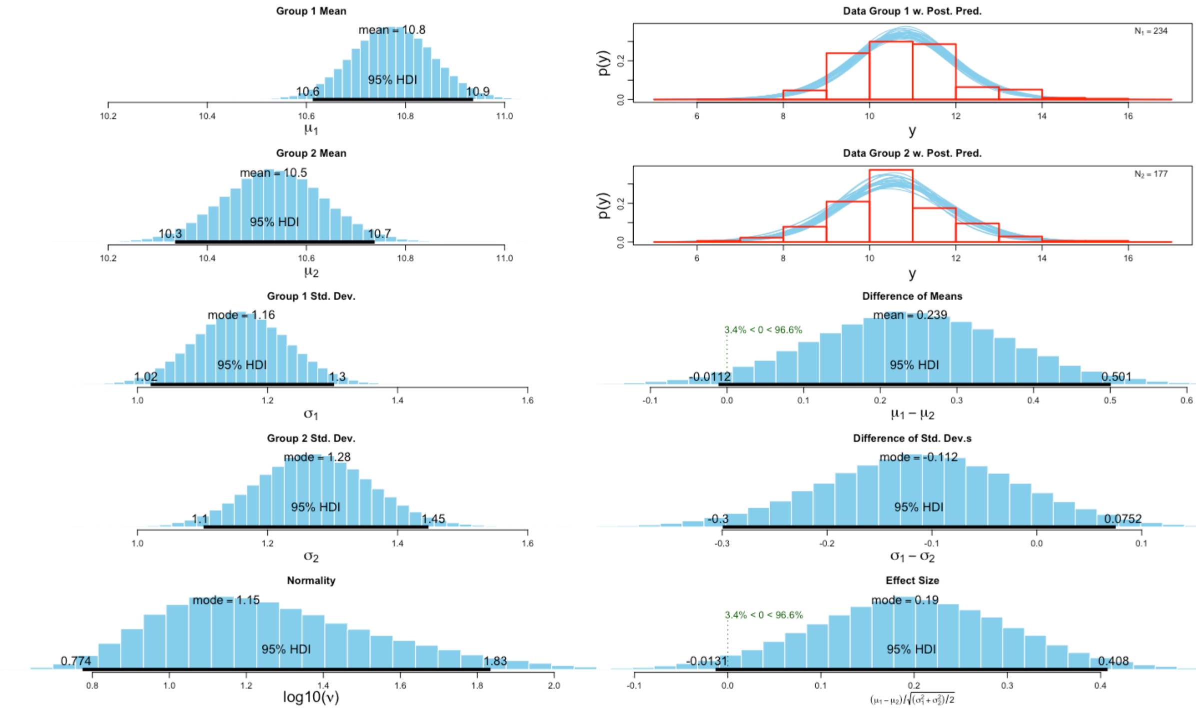


Figure D-26: BEST test output for females (group 1) vs males (group 2) dentine $\delta^{15}N_{coll}$ values in England.

D.iv.i Outputs for enamel $\delta^{13}C$, bone and dentine in England by sex and time period

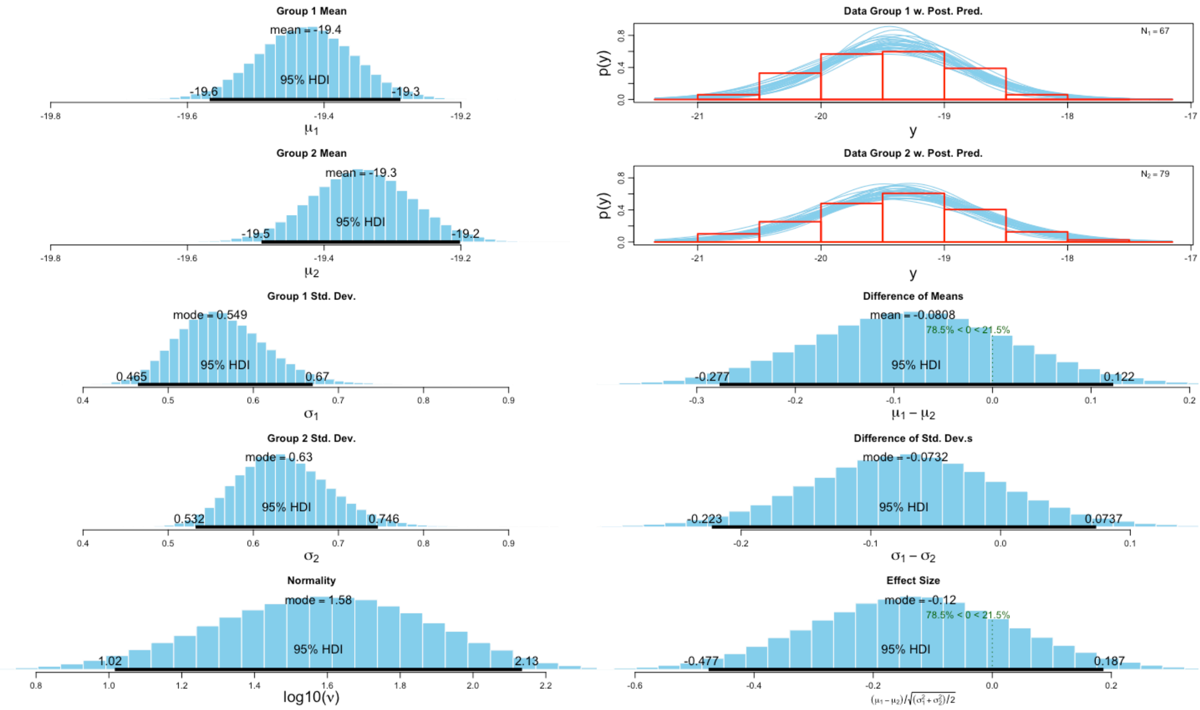


Figure D-27: BEST test output for females (group 1) vs males (group 2) bone $\delta^{13}C_{coll}$ values in England c. 200BC-450 AD.

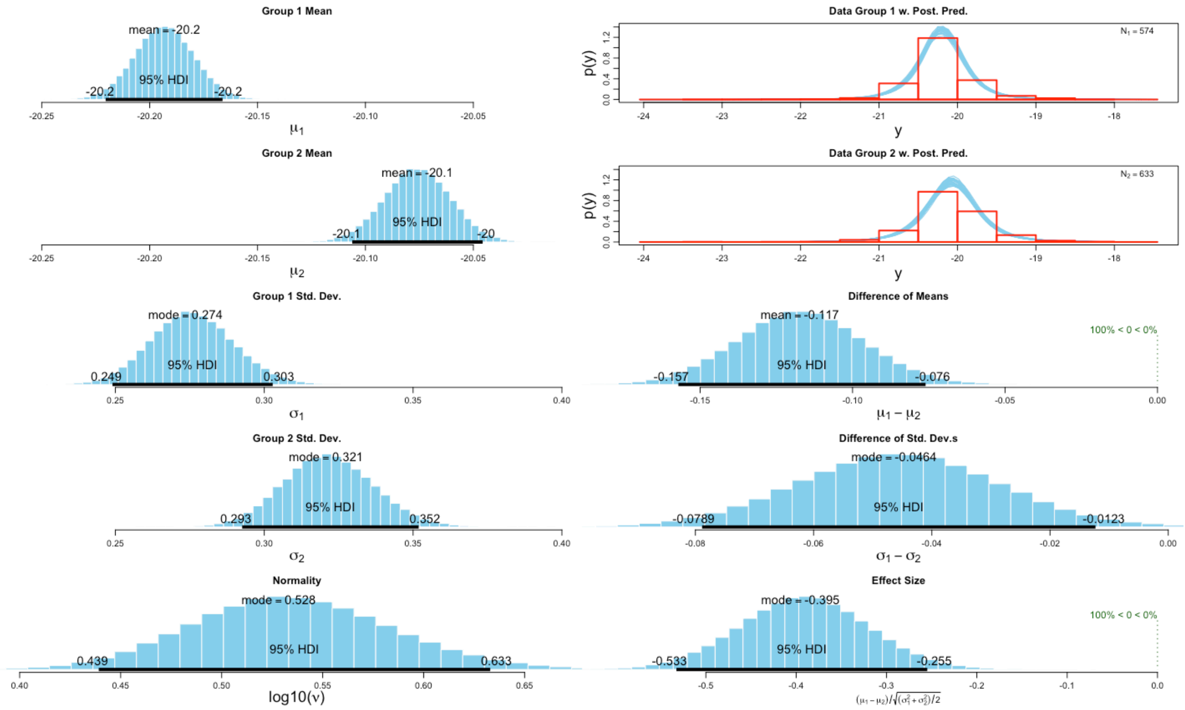


Figure D-28: BEST test output for females (group 1) vs males (group 2) bone δ13Ccoll values in England c. 450-790 AD.

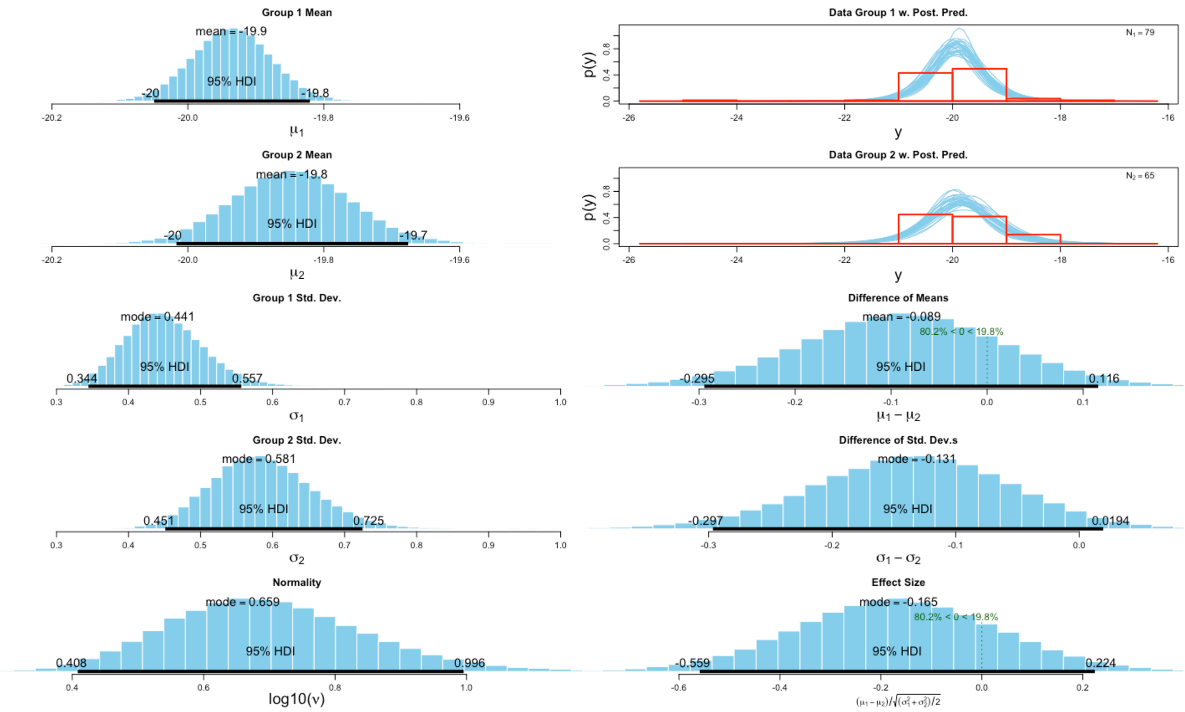


Figure D-29: BEST test output for females (group 1) vs males (group 2) bone δ13Ccoll values in England c. 790-1066+ AD.

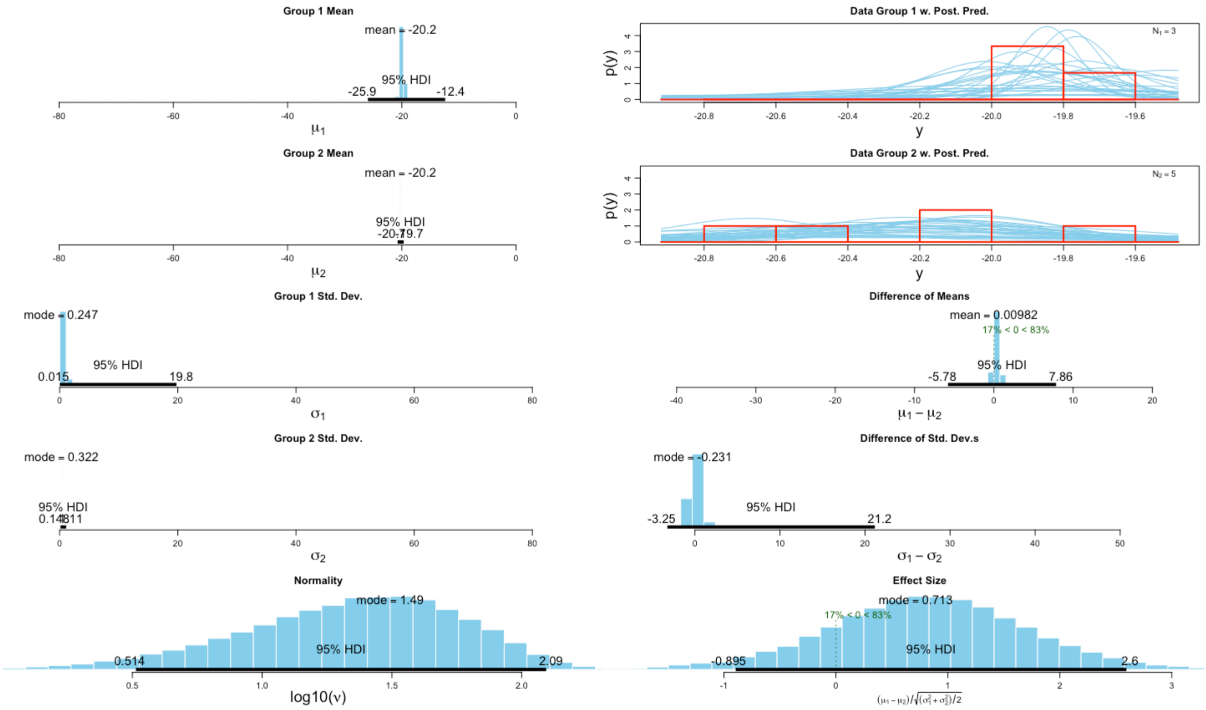


Figure D-30: BEST test output for females (group 1) vs males (group 2) dentine δ13Ccoll values in England c. 200BC-450 AD.

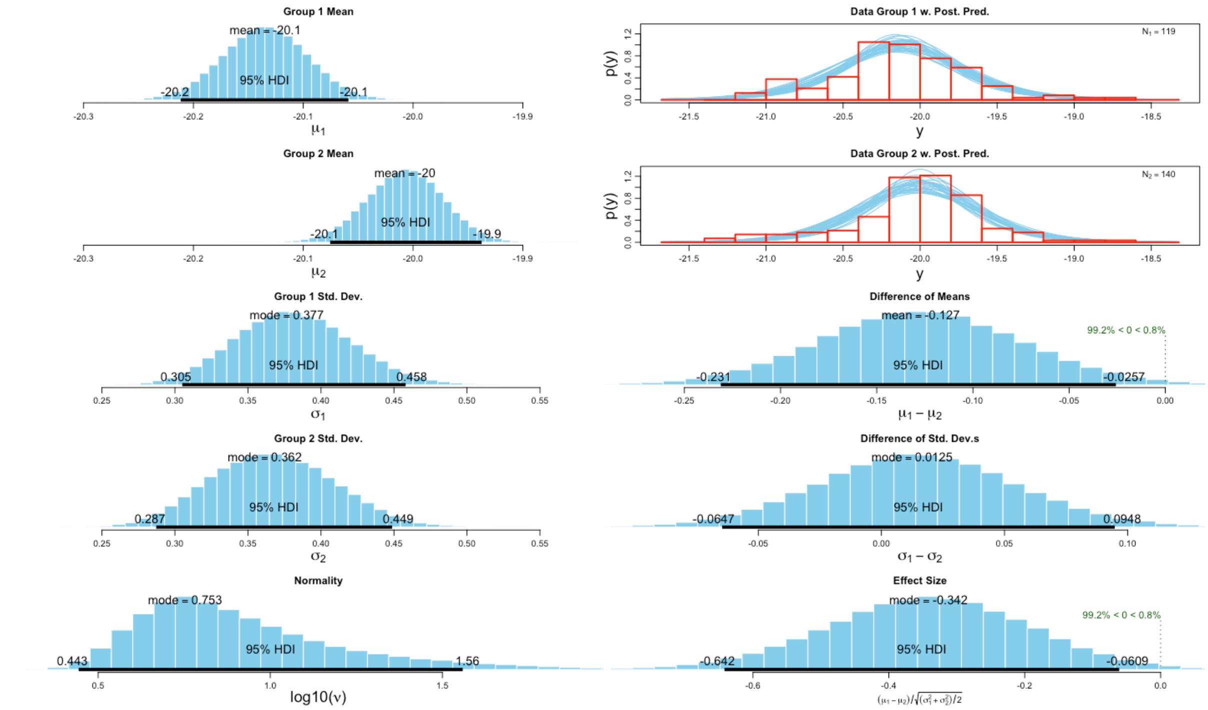


Figure D-31: BEST test output for females (group 1) vs males (group 2) dentine δ13Ccoll values in England c. 450-790 AD.

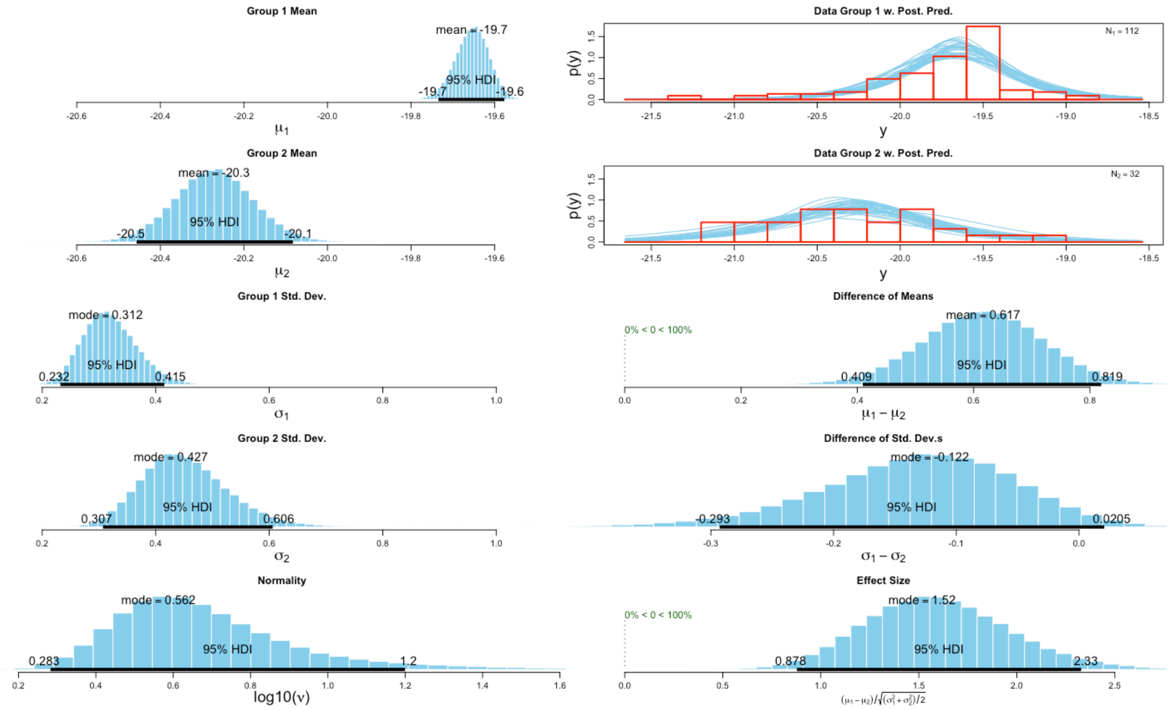


Figure D-32: BEST test output for females (group 1) vs males (group 2) dentine $\delta^{13}C_{coll}$ values in England c. 790-1066+ AD.

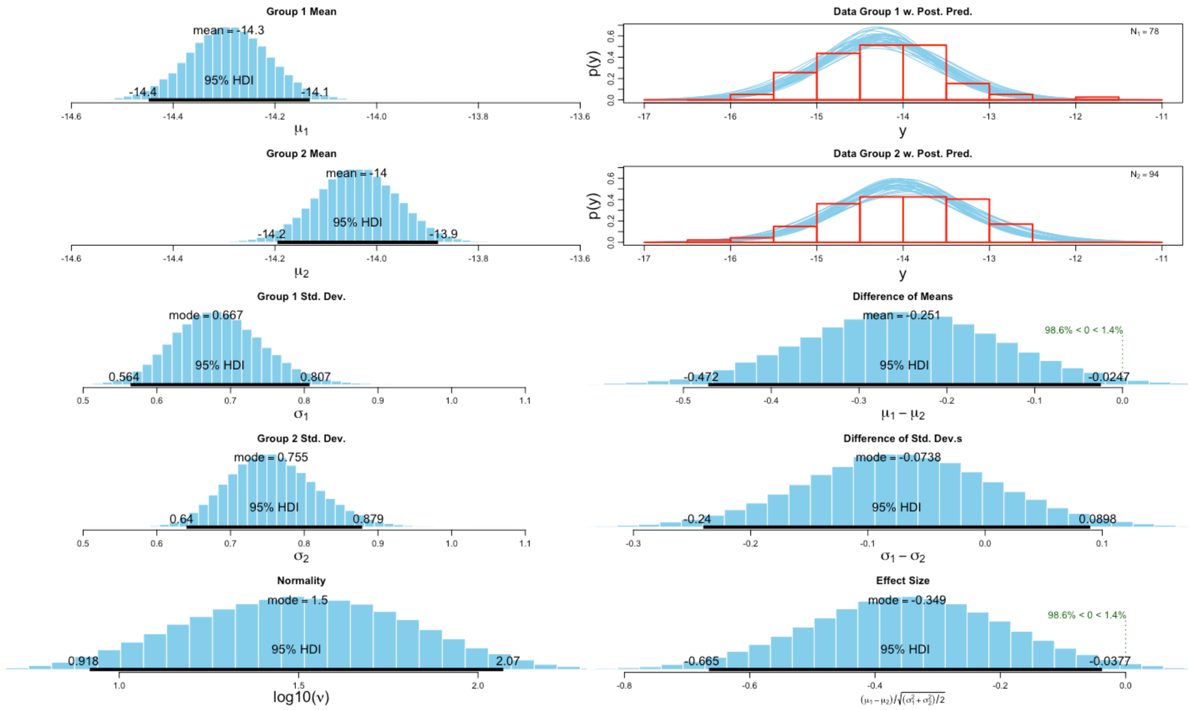


Figure D-33: BEST test output for females (group 1) vs males (group 2) enamel $\delta^{13}C_{carb}$ values in England c. 450-790 AD.

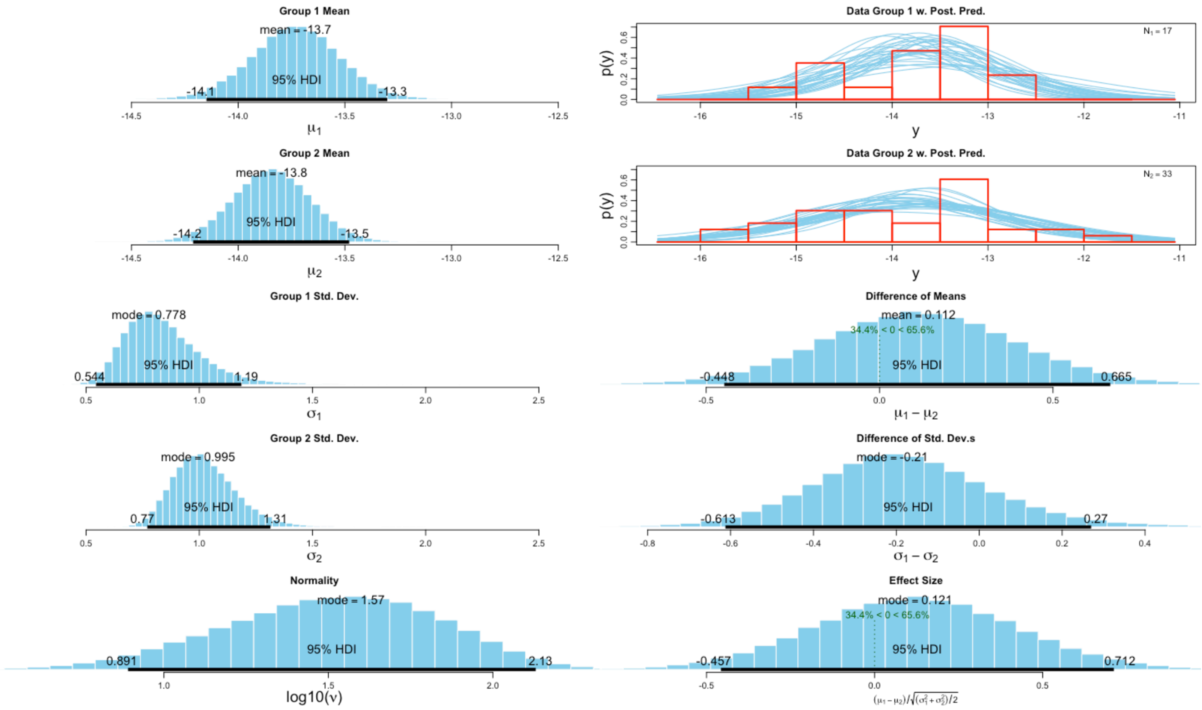


Figure D-34: BEST test output for females (group 1) vs males (group 2) enamel $\delta^{13}C_{carb}$ values in England c. 790-1066+ AD.

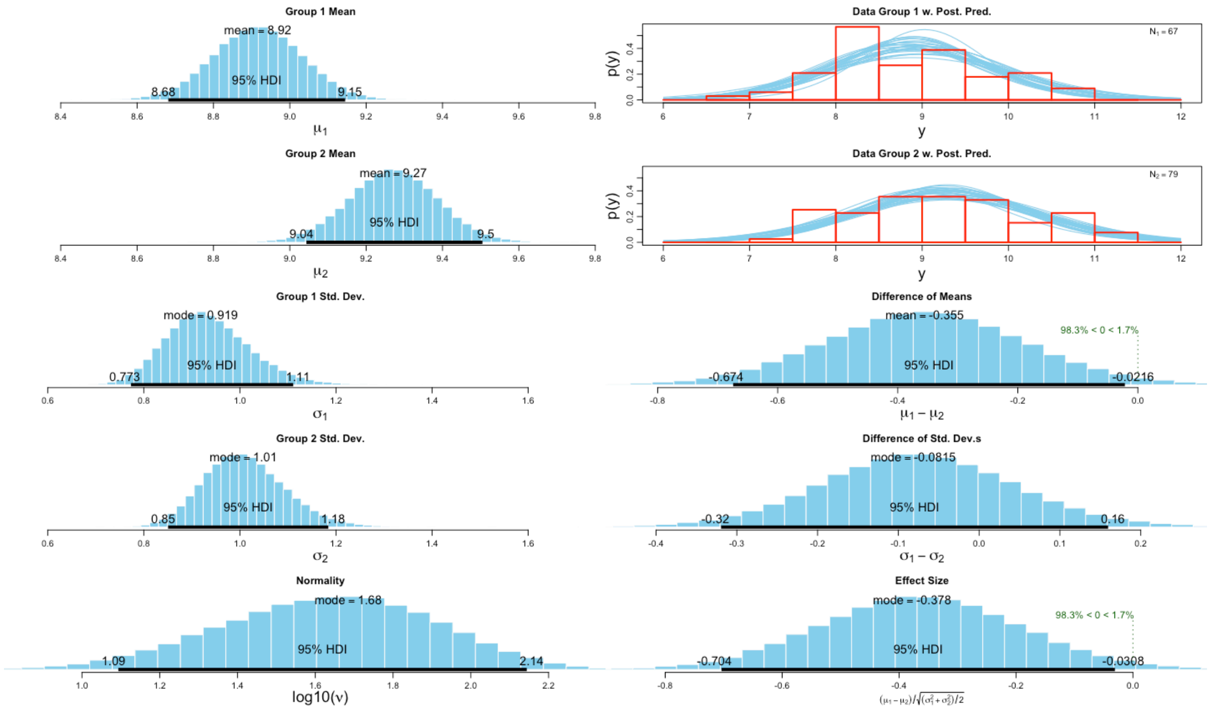


Figure D-35: BEST test output for females (group 1) vs males (group 2) bone $\delta^{15}N_{coll}$ values in England c. 200 BC - 450 AD.

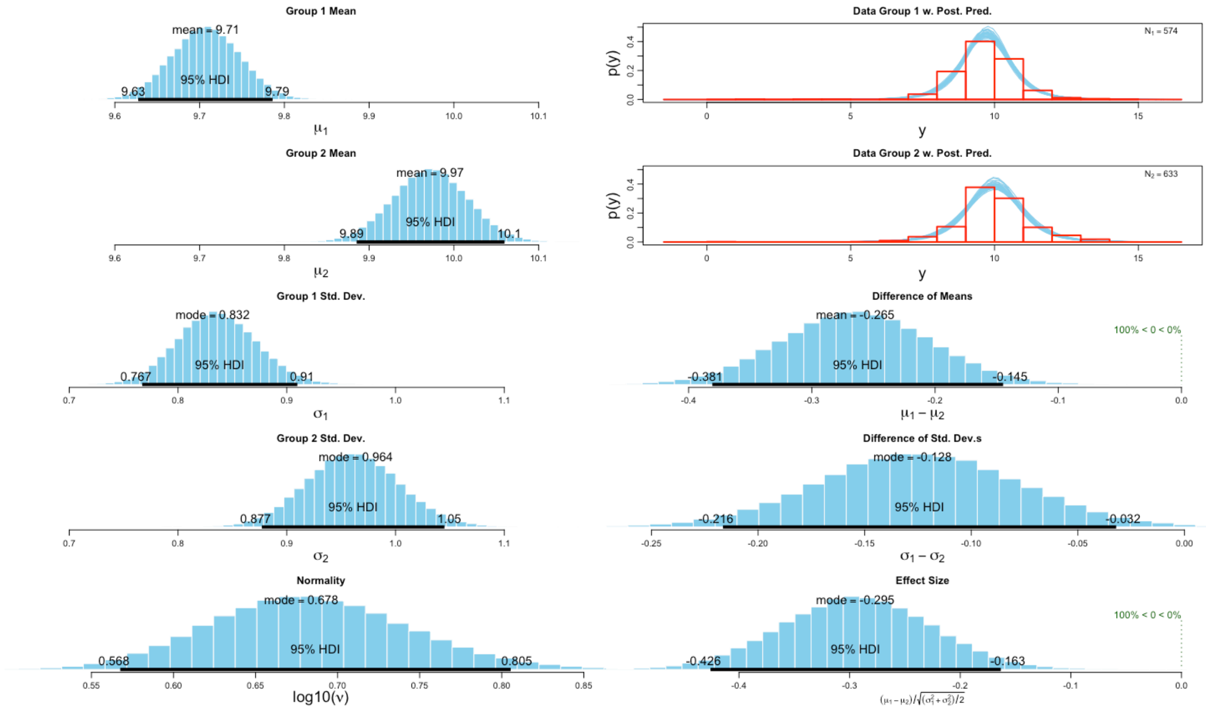


Figure D-36: BEST test output for females (group 1) vs males (group 2) bone $\delta^{15}N_{coll}$ values in England c. 450-790 AD.

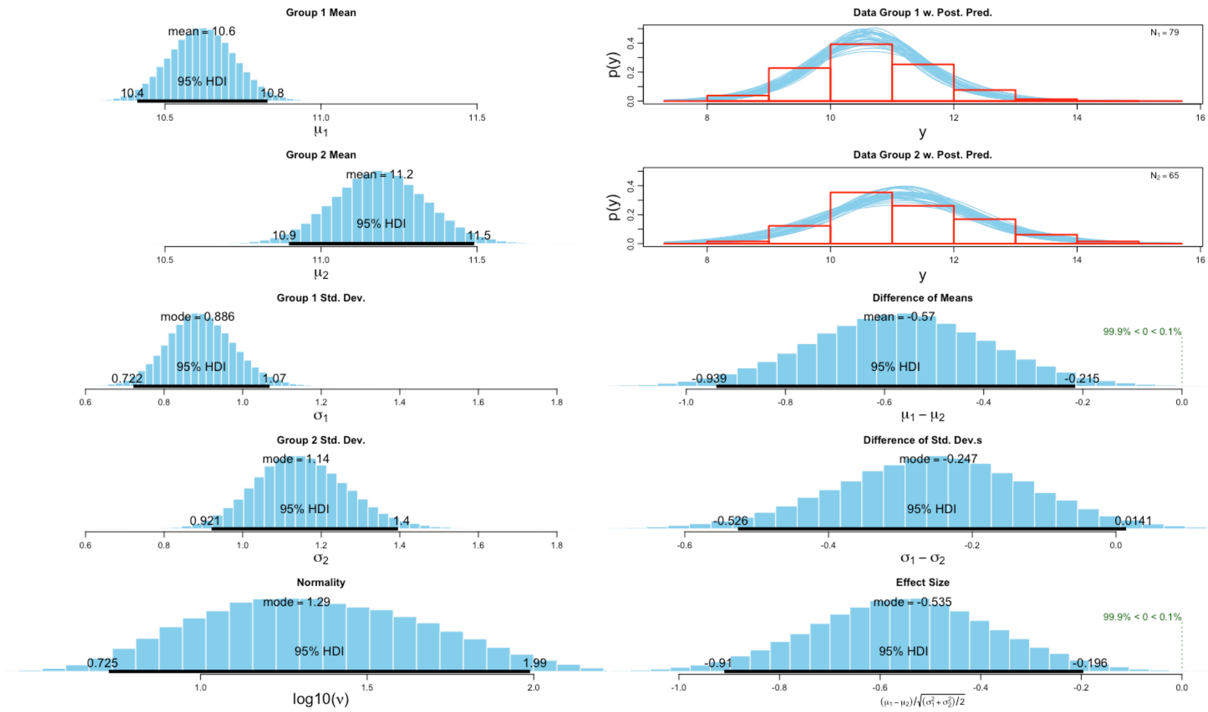


Figure D-37: BEST test output for females (group 1) vs males (group 2) bone $\delta^{15}N_{coll}$ values in England c. 790-1066+ AD.

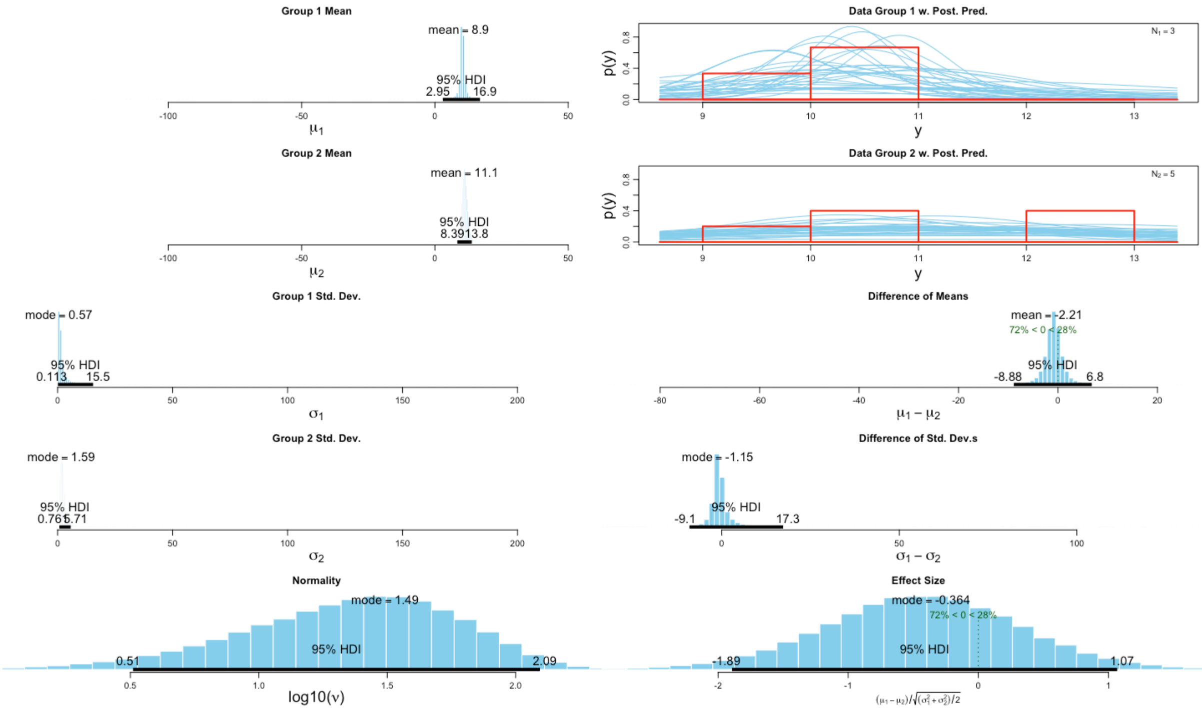


Figure D-38: BEST test output for females (group 1) vs males (group 2) dentine $\delta^{15}N_{coll}$ values in England c. 200 BC - 450 AD.

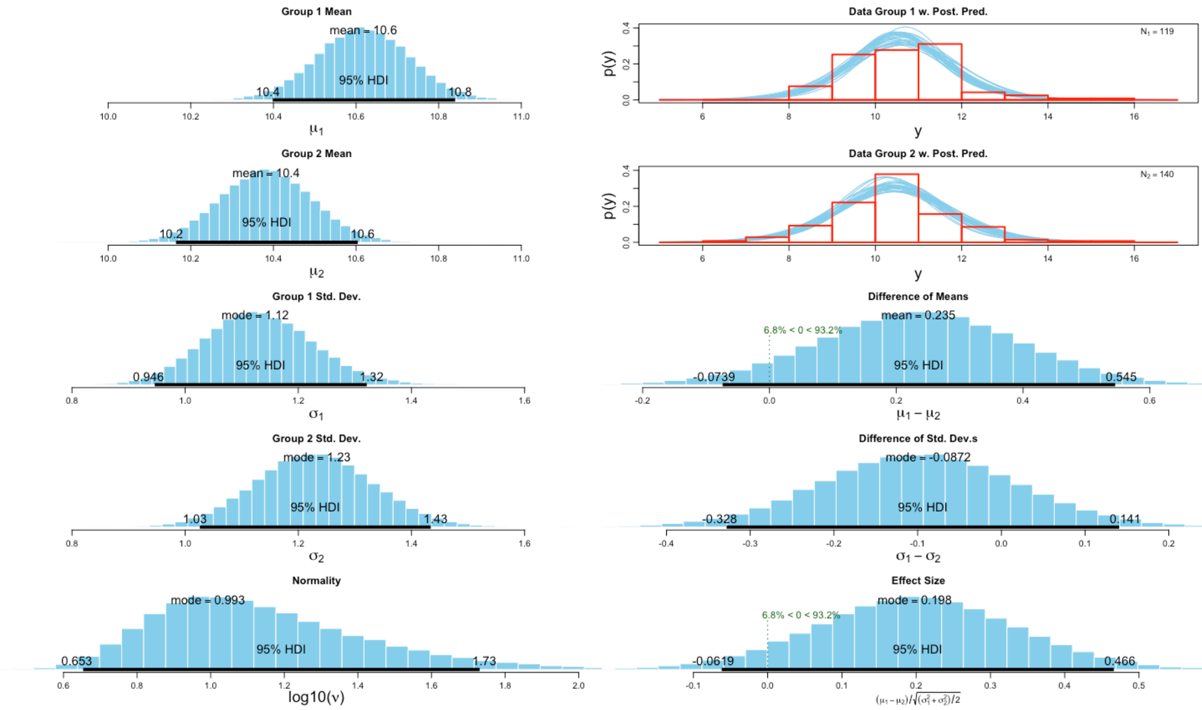


Figure D-39: BEST test output for females (group 1) vs males (group 2) dentine $\delta^{15}N_{coll}$ values in England c. 450-790 AD.

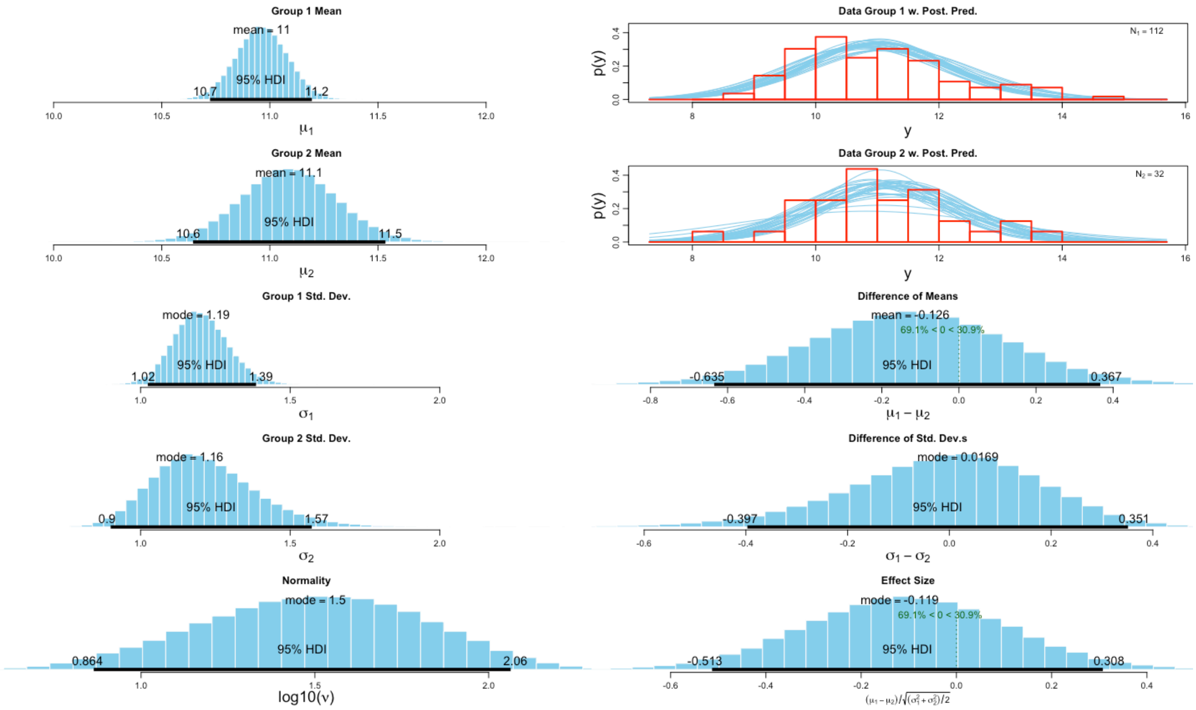


Figure D-40: BEST test output for females (group 1) vs males (group 2) dentine $\delta^{15}N_{coll}$ values in England c. 790-1066+ AD.

D.v Outputs for matched bone and dentine

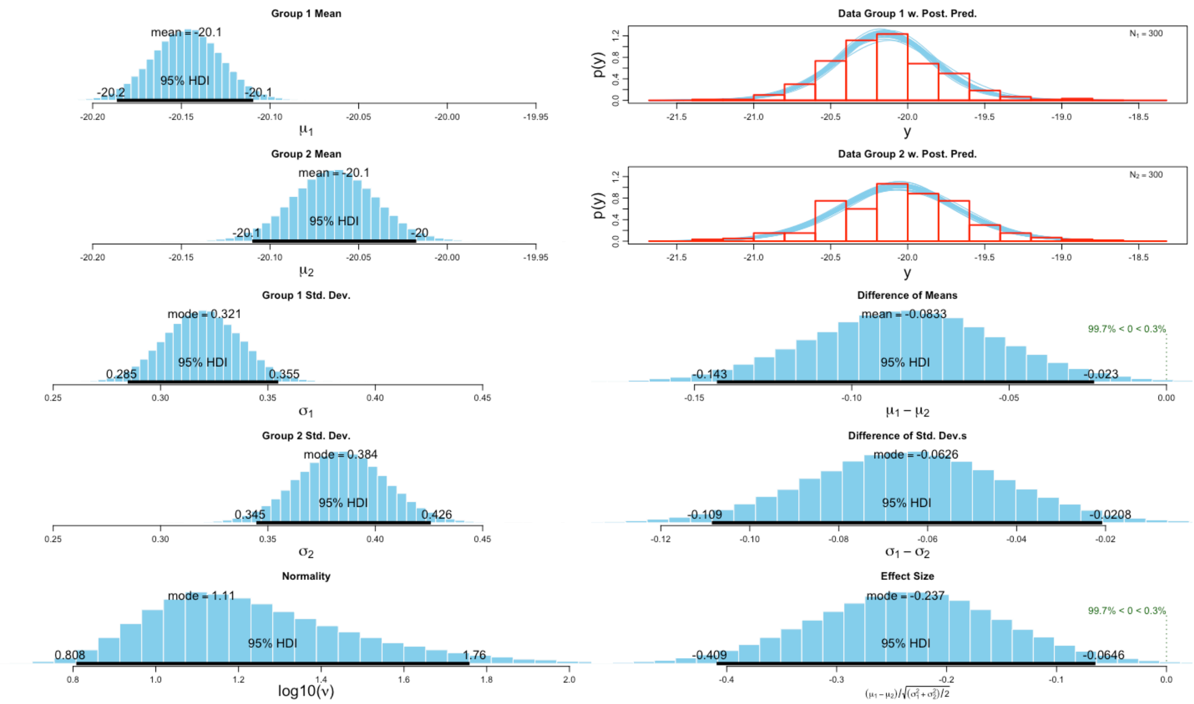


Figure D-41: BEST test output for matched bone (group 1) vs dentine (group 2) for $\delta^{13}C_{coll}$ values in England (all age groups).

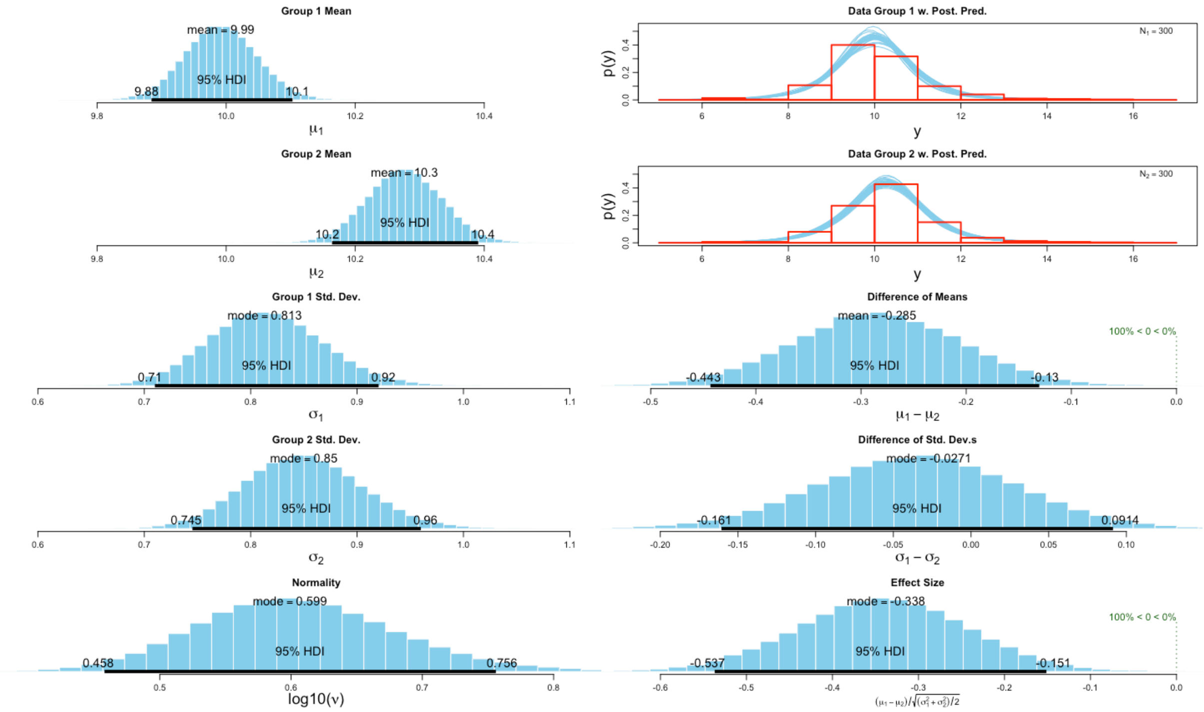


Figure D-42: BEST test output for matched bone (group 1) vs dentine (group 2) for $\delta^{15}N_{coll}$ values in England (all age groups).

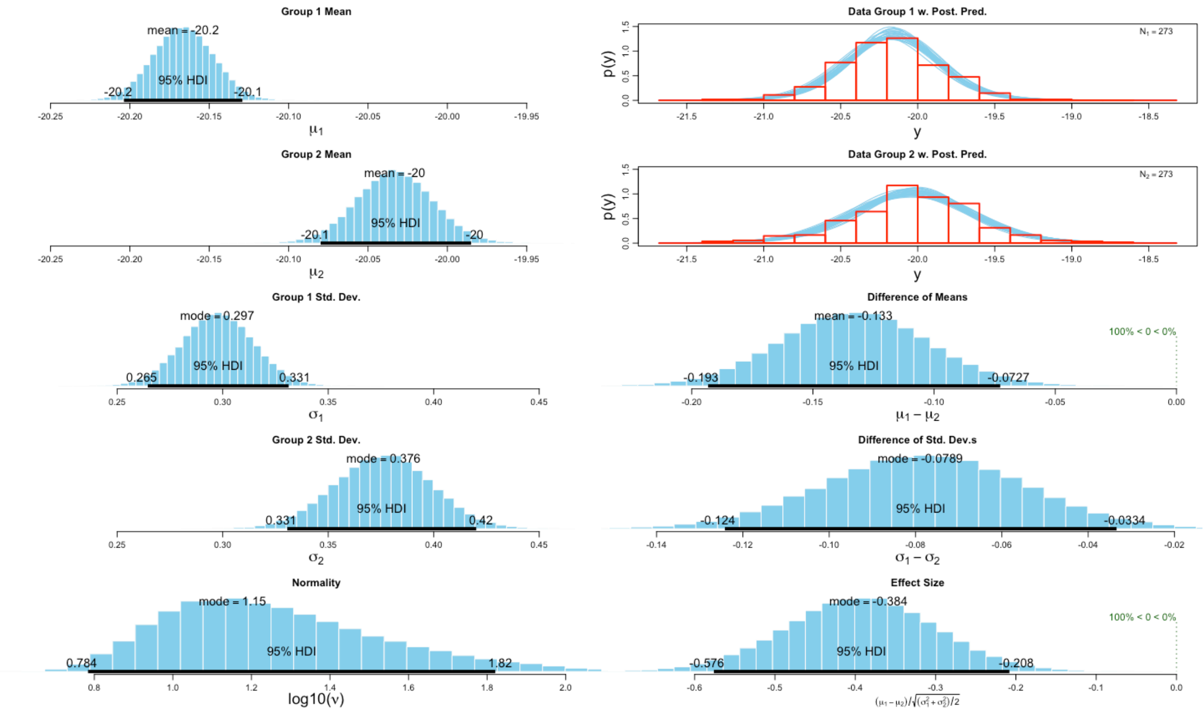


Figure D-43: BEST test output for matched bone (group 1) vs dentine (group 2) for $\delta^{13}C_{coll}$ values in England (age category 3 and up).

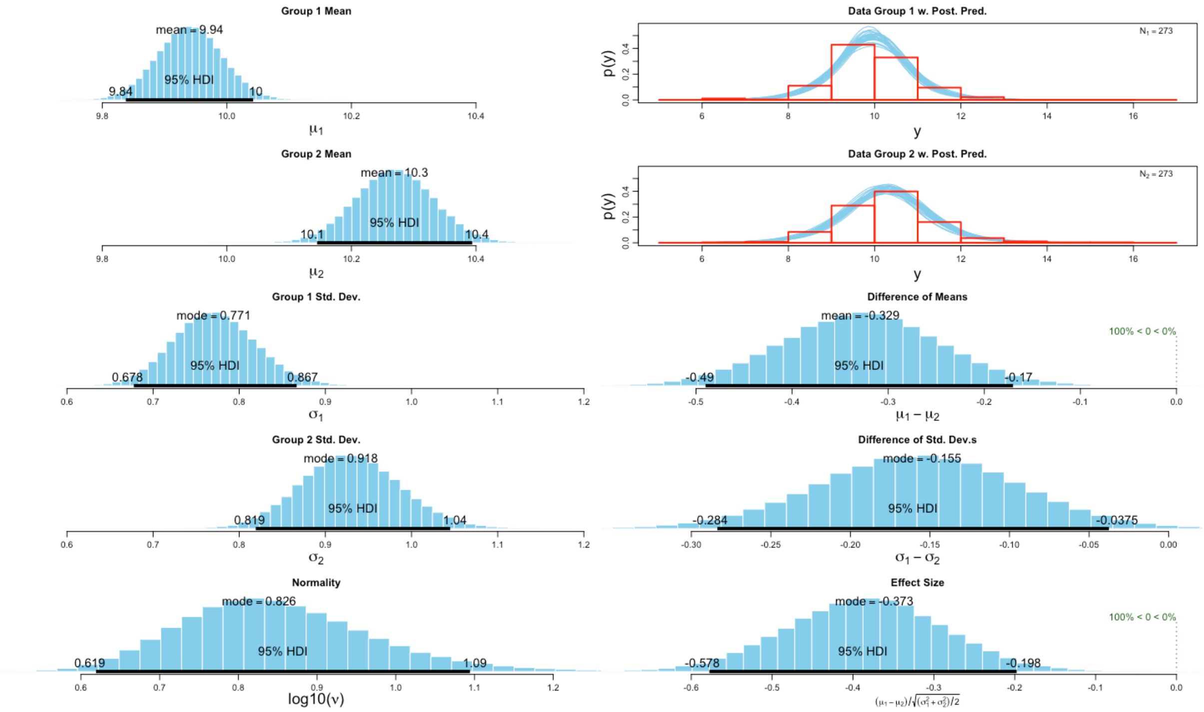


Figure D-44: BEST test output for matched bone (group 1) vs dentine (group 2) for $\delta^{15}N_{coll}$ values in England (age category 3 and up).

D.vi Outputs for Kent and East Sussex

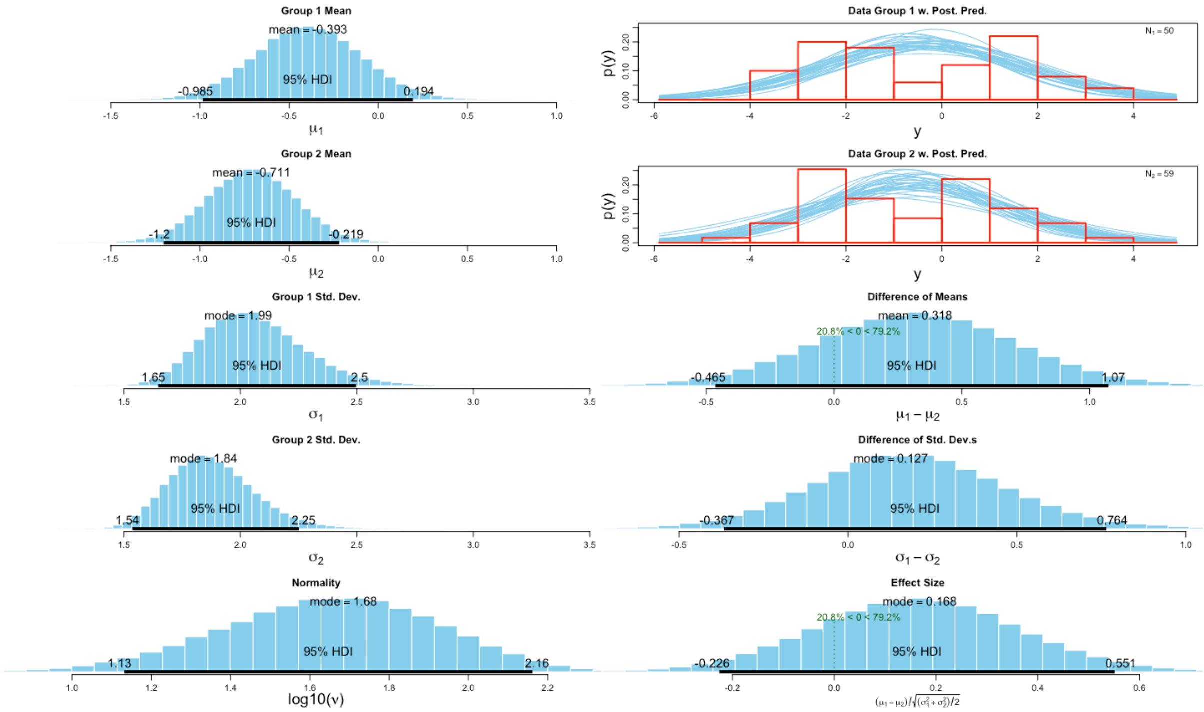


Figure D-45: BEST test output for females (group 1) vs males (group 2) for $\Delta^{18}O_{dw\text{-}MAP\ (Chenery)}$ values in Kent and East Sussex.

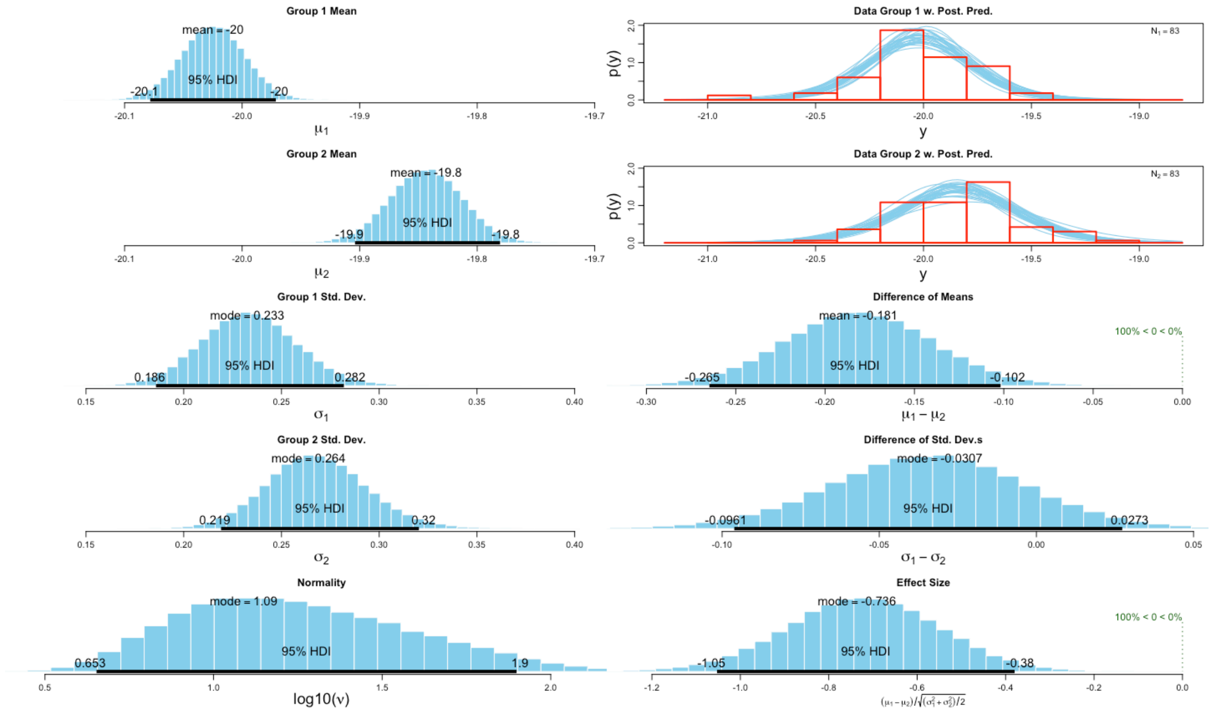


Figure D-46: BEST test output for matched bone (group 1) vs dentine (group 2) for $\delta^{13}C_{coll}$ values in Kent and East Sussex.

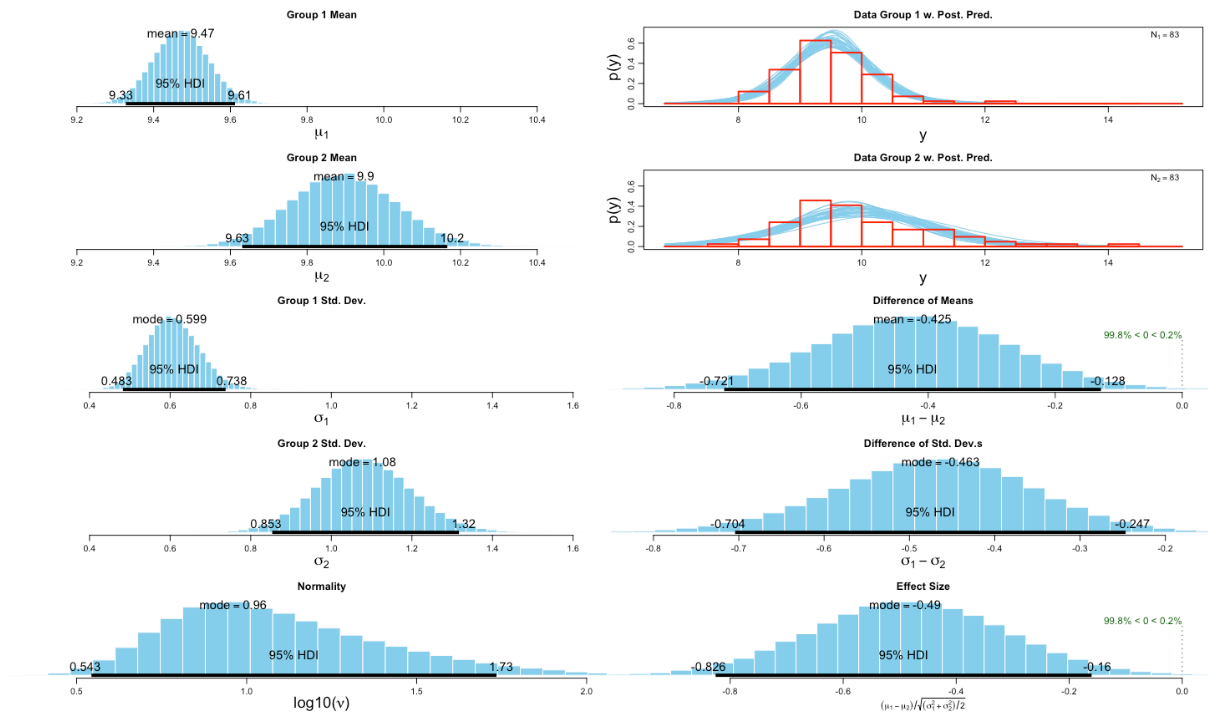


Figure D-47: BEST test output for matched bone (group 1) vs dentine (group 2) for $\delta^{15}N_{coll}$ values in Kent and East Sussex.

D.vii Outputs for Finglesham

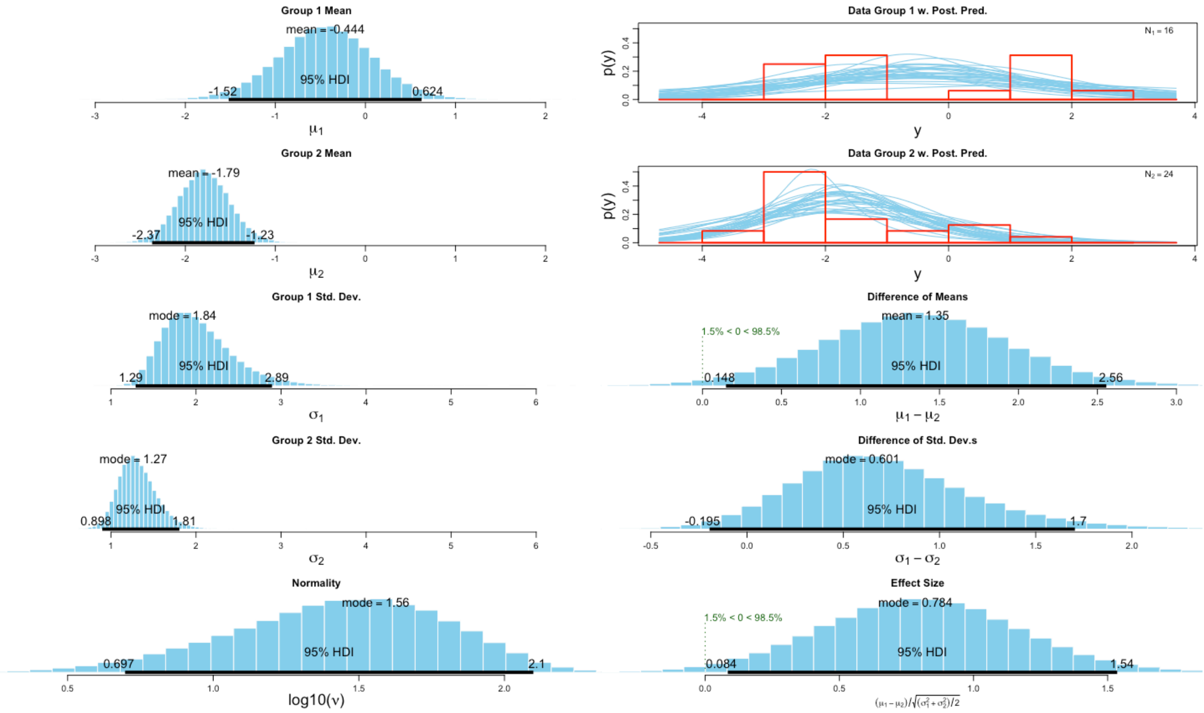


Figure D-48: BEST test output for females (group 1) vs males (group 2) for $\Delta^{18}O_{dw\text{-}MAP\ (Chenery)}$ values in Finglesham.

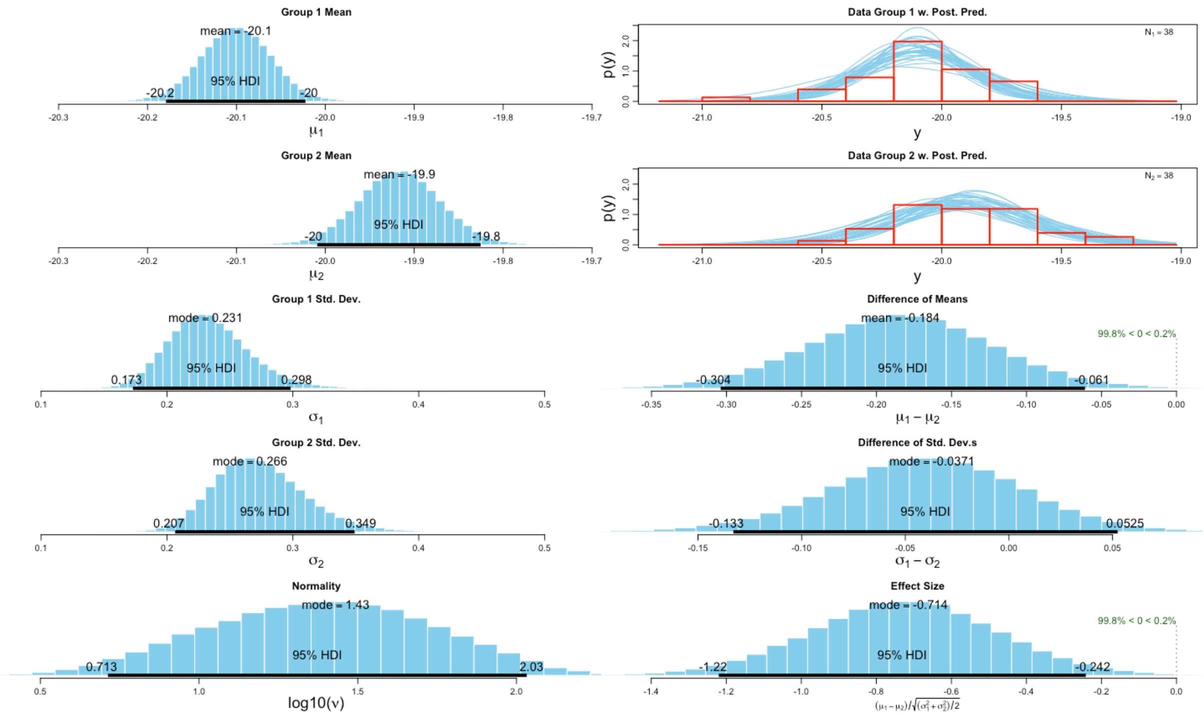


Figure D-49: BEST test output for matched bone (group 1) vs dentine (group 2) for $\delta^{13}C_{coll}$ values in Finglesham.

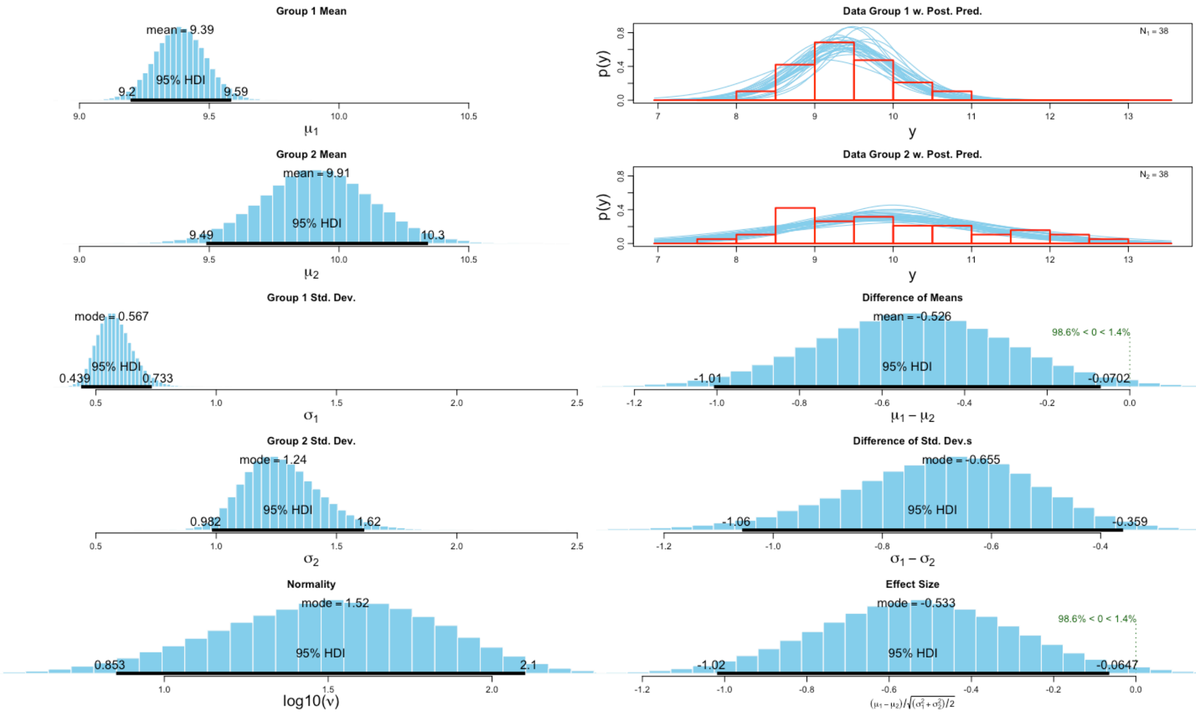


Figure D-50: BEST test output for matched bone (group 1) vs dentine (group 2) for $\delta^{15}N_{coll}$ values in Finglesham.

E Linear Model Outputs and Conversion Comparisons

E.i Comparisons of Levison vs. Chenery on $\Delta^{18}O_{dw\text{-}MAP}$ value distributions and outliers

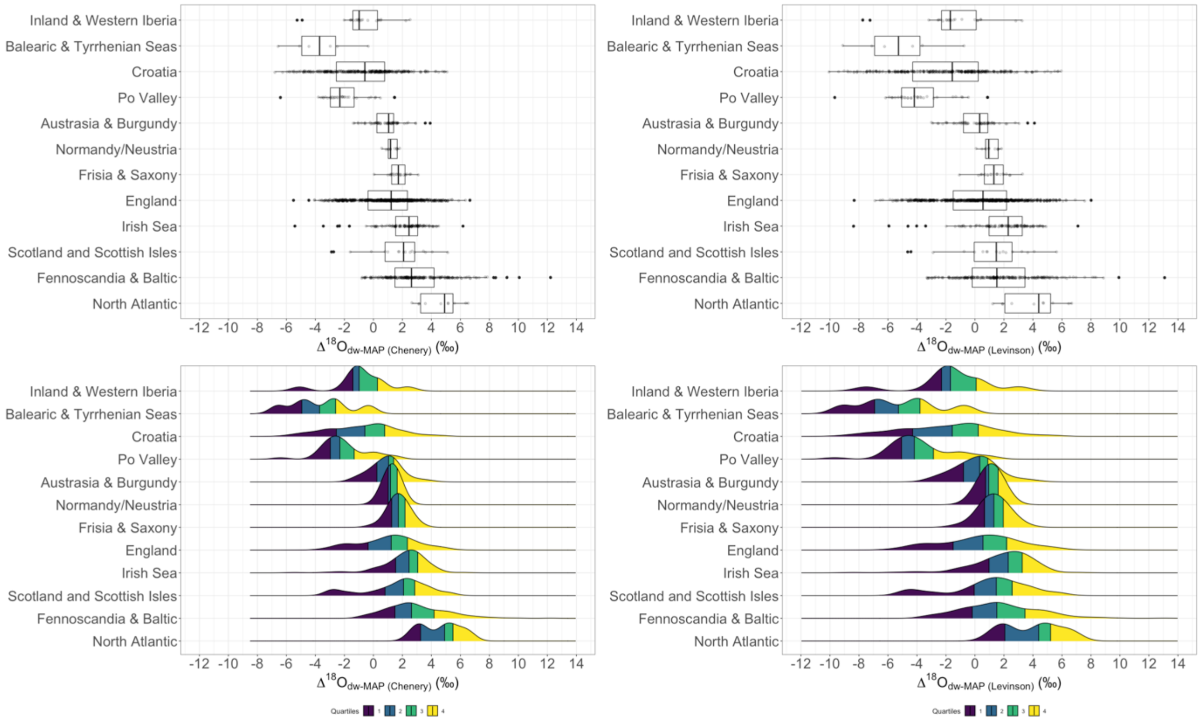


Figure E-1: Comparisons of Levison vs. Chenery on $\Delta^{18}O_{dw\text{-}MAP}$ value distributions and outliers for European regions.

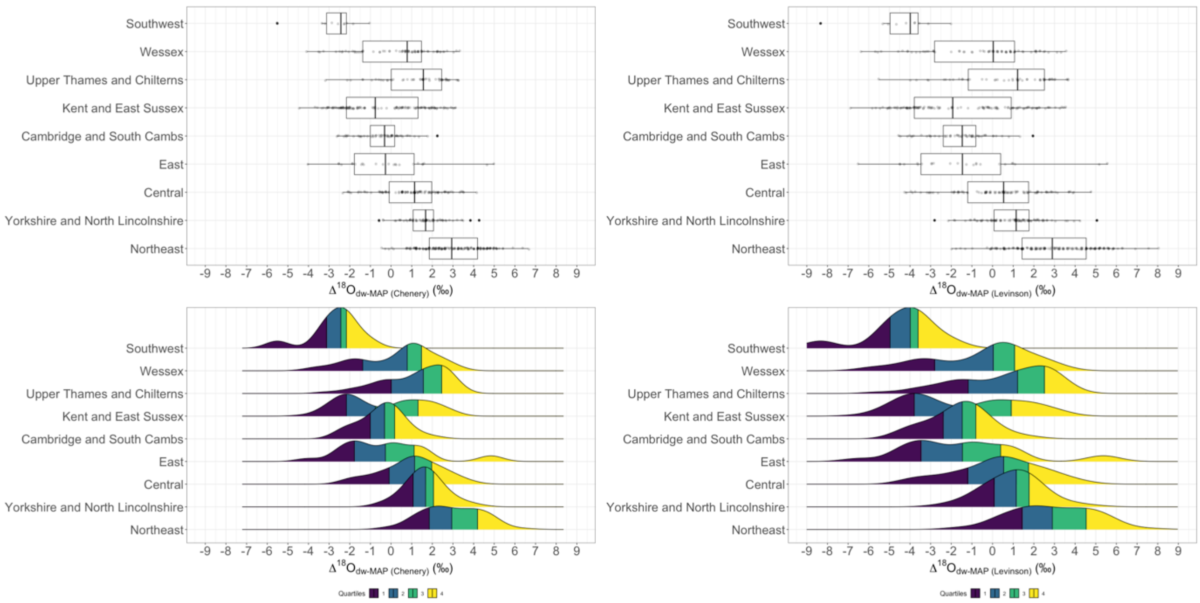


Figure E-2 Comparisons of Levison vs. Chenery on $\Delta^{18}O_{dw\text{-}MAP}$ value distributions and outliers for regions in England.

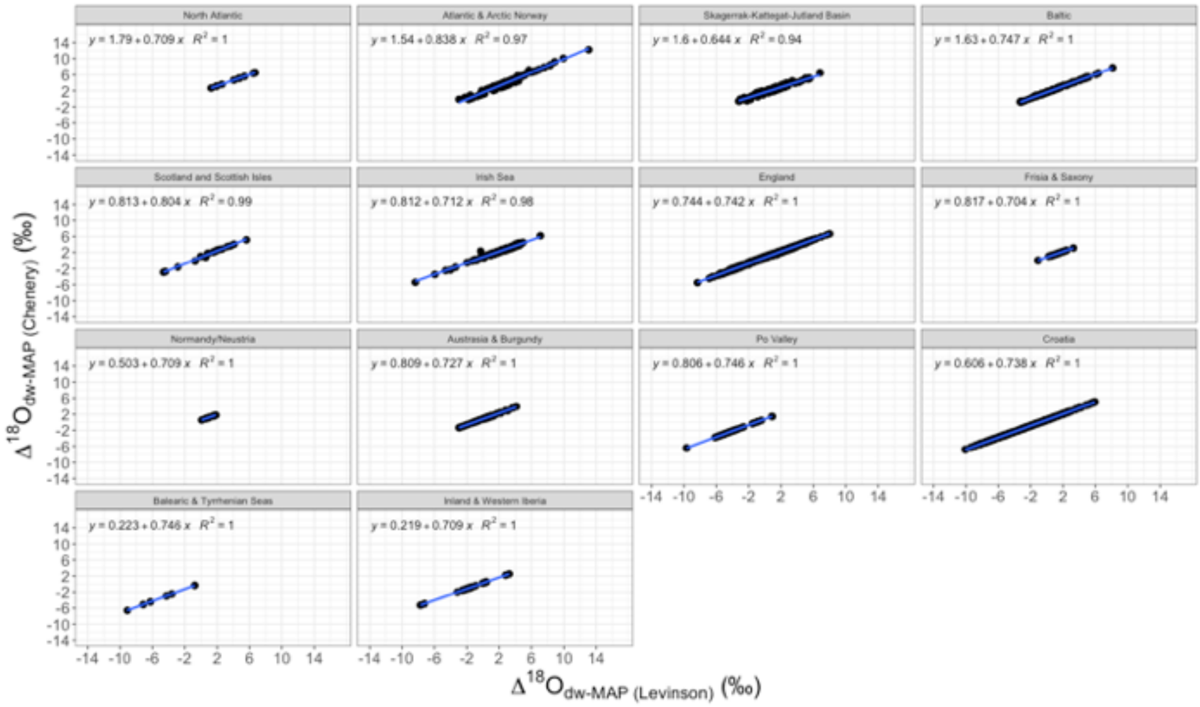


Figure E-3: Comparisons of Levison vs. Chenery on $\Delta^{18}O_{dw\text{-}MAP}$ values by European regions, individualised linear models with line equations.

Region	Line Equation	R^2 value
All of Early Medieval Europe	y=0.856+0.779x	0.97
North Atlantic	y=1.79+0.709x	1
Arctic and Atlantic Norway	y=1.54+0.838x	0.97
Skagerrak-Kattegat-Jutland Basin	y=1.6+0.644x	0.94
Baltic	y=1.63+0.747x	1
Scotland and Scottish Isles	y=0.813+0.804x	0.99
Irish Sea	y=0.812+0.712x	0.98
England	y=0.744+0.742x	1
Frisia & Saxony	y=0.817+0.704x	1
Normandy/Neustria	y=0.503+0.709x	1
Austrasia &Burgundy	y=0.809+0.727x	1
Po Valley	y=0.806+0.746x	1
Croatia	y=0.606+0.738x	1
Balearic & Tyrrhenian Seas	y=0.223+0.746x	1
Inland & Western Iberia	y=0.219-0.709x	1

Table E-1: Line equations and R^2 values for Early Medieval European comparing $\Delta^{18}O_{dw\text{-}MAP}$ values for both conversion methods by region as per Figure E-3.

E.ii Comparison between $\varepsilon^{13}C$ and $\Delta^{13}C$

Epsilon values don't make much difference, both are almost perfect linear relationships – see below.

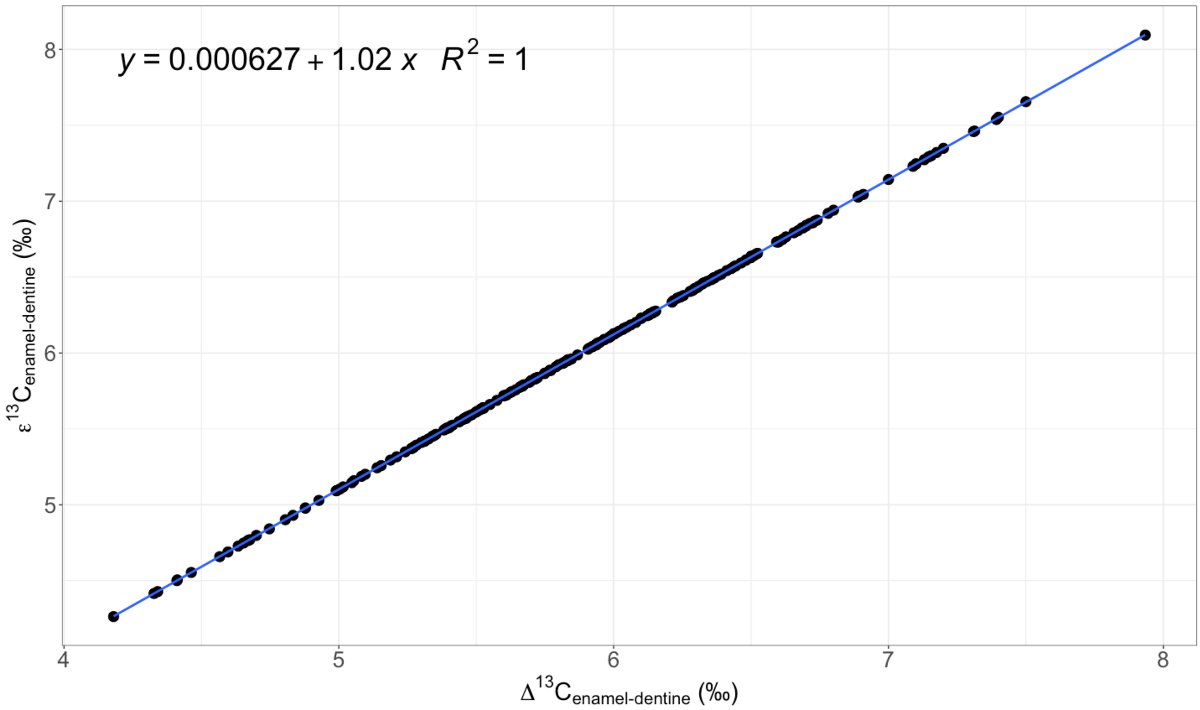


Figure E-4: $\Delta^{13}C_{enamel\text{-}dentine}$ versus $\varepsilon^{13}C_{enamel\text{-}dentine}$ values from human data in Early Medieval England.

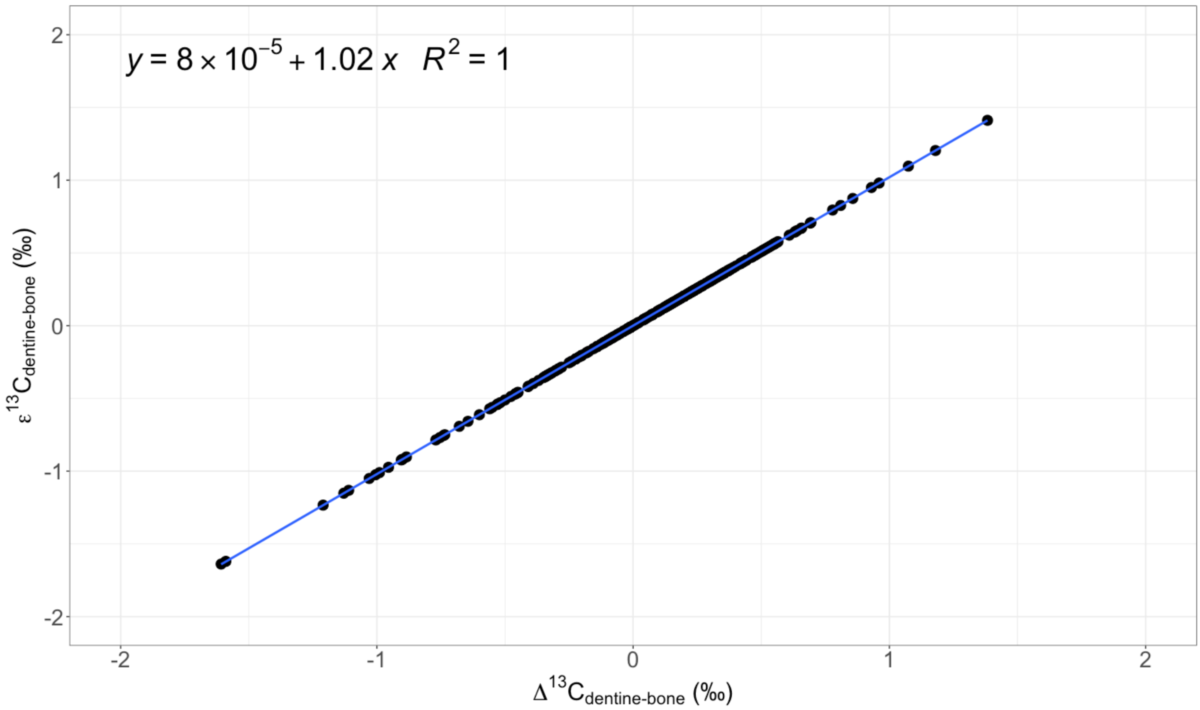


Figure E-5: $\Delta^{13}C_{dentine\text{-}bone}$ versus $\varepsilon^{13}C_{dentine\text{-}bone}$ values from human data in Early Medieval England.

F Hierarchical Cluster Validation Indices

F.i Enamel Combination 1 (O, C, Sr)

NbClust(data = enamelclean, diss = NULL, distance = "euclidean", min.nc = 2, max.nc = 15, method = "ward.D2")

*** : The Hubert index is a graphical method of determining the number of clusters.
In the plot of Hubert index, we seek a significant knee that corresponds to a significant increase of the value of the measure i.e the significant peak in Hubert
index second differences plot.

*** : The D index is a graphical method of determining the number of clusters.
In the plot of D index, we seek a significant knee (the significant peak in Dindex
second differences plot) that corresponds to a significant increase of the value of
the measure.

****
* Among all indices:
* 8 proposed 2 as the best number of clusters
* 6 proposed 3 as the best number of clusters
* 5 proposed 4 as the best number of clusters
* 2 proposed 5 as the best number of clusters
* 1 proposed 11 as the best number of clusters
* 1 proposed 14 as the best number of clusters
* 1 proposed 15 as the best number of clusters

***** Conclusion *****

* According to the majority rule, the best number of clusters is 2

****

$All.index

	KL	CH	Hartigan	CCC	Scott	Marriot	TrCovW	TraceW	Friedman	Rubin	Cindex	DB	Silhouette	Duda
2	0.1541	156.3133	140.8910	0.4316	472.1498	12235252	49442.918	517.6715	4.3350	1.6323	0.2704	0.8006	0.5040	0.6348
3	2.3717	187.1209	81.4100	1.5286	765.9459	9748395	21085.730	344.7945	6.4886	2.4507	0.2314	1.1375	0.3594	0.5668
4	3.3568	187.4822	51.1928	3.4621	915.0431	10233040	10342.397	267.1273	7.4198	3.1633	0.2840	1.0506	0.3596	0.6582
5	1.9959	178.5679	32.8307	3.5453	1051.5002	9872255	6720.973	225.7121	8.7511	3.7437	0.2582	1.1100	0.2963	0.6415
6	0.9245	165.6928	26.7376	2.8183	1138.8970	10438999	4989.475	201.8718	10.0838	4.1858	0.2415	1.1403	0.2835	0.7037
7	1.5251	155.2990	23.6211	2.1809	1228.1339	10365938	4138.681	184.1013	11.8076	4.5899	0.2246	1.2063	0.2863	0.6726
8	2.6690	147.3444	21.6993	1.7118	1303.4290	10376332	3707.391	169.5874	13.5747	4.9827	0.2172	1.2359	0.2635	0.5678

9 0.2879 141.2962 22.5864 1.3957 1353.0961 11018674 2910.180 157.1845
14.1669 5.3759 0.2090 1.2345   0.2328 0.6592
10 0.9239 137.9541 20.7745 1.4021 1410.0089 11125139 2394.224 145.2142
14.8384 5.8190 0.2011 1.2323   0.2393 0.5673
11 0.7104 135.1872 20.2968 1.4337 1478.1394 10581254 2066.628 134.9453
16.9373 6.2618 0.1910 1.1727   0.2452 0.9168
12 1.0047 133.4209 18.9103 1.5727 1532.7282 10383450 1741.335 125.5748
17.7234 6.7291 0.2506 1.0775   0.2526 0.5565
13 1.3902 131.9240 16.5999 1.7136 1592.9097 9851692 1467.747 117.3838
18.8410 7.1986 0.2430 1.0393   0.2581 0.4771
14 0.8738 130.0564 16.0257 1.7587 1649.8063 9344718 1300.296 110.5850
21.0367 7.6412 0.2378 1.0248   0.2627 0.6521
15 0.9170 128.6261 15.4746 1.8440 1702.4163 8907520 1112.950 104.3673
22.4241 8.0964 0.2422 1.0626   0.2587 0.5919
  Pseudot2 Beale Ratkowsky   Ball Ptbiserial   Frey McClain   Dunn Hubert SDindex
Dindex   SDbw
2 143.2688 0.9756   0.2834 258.8358   0.6301 2.3784 0.1230 0.0826 0.0033
2.0966 1.2020 0.6722
3   81.0137 1.2890   0.3769 114.9315   0.5455 0.3897 0.7318 0.0364 0.0029 2.2958
0.9776 0.7368
4   73.2185 0.8778   0.3948 66.7818   0.5627 1.7598 0.8879 0.0500 0.0031 2.1626
0.8693 0.6697
5   38.0022 0.9376   0.3730 45.1424   0.4598 0.3584 1.6421 0.0399 0.0033 2.6682
0.7854 0.6850
6   32.8476 0.7079   0.3473 33.6453   0.4538 0.6614 1.8261 0.0399 0.0035 2.6120
0.7417 0.4981
7   14.6007 0.8018   0.3263 26.3002   0.4234 0.0926 2.2640 0.0376 0.0037 2.7750
0.7081 0.4593
8   35.0109 1.2682   0.3079 21.1984   0.4261 0.4879 2.2836 0.0376 0.0039 2.7531
0.6795 0.5777
9   18.6134 0.8564   0.2946 17.4649   0.4141 0.1170 2.4840 0.0376 0.0039 2.9043
0.6435 0.5033
10 35.8537 1.2716   0.2835 14.5214   0.4154 0.2356 2.5121 0.0376 0.0040 3.1031
0.6250 0.4827
11   1.9052 0.1474   0.2718 12.2678   0.4108 -0.0535 2.6216 0.0376 0.0040 3.1537
0.6000 0.3866
12 23.1146 1.3117   0.2630 10.4646   0.4133 0.2661 2.5984 0.0500 0.0041 2.8314
0.5891 0.2671
13 28.4943 1.7966   0.2549   9.0295   0.4095 0.3732 2.6716 0.0500 0.0041 2.8114
0.5693 0.3196
14 10.6721 0.8652   0.2465   7.8989   0.4045 0.1383 2.7536 0.0500 0.0041 2.8376
0.5503 0.2607
15 13.7897 1.1179   0.2394   6.9578   0.4041 0.1975 2.7700 0.0522 0.0042 2.8099
0.5388 0.2446

$All.CriticalValues
  CritValue_Duda CritValue_PseudoT2 Fvalue_Beale
2   0.6469   135.9091   0.4036
3   0.5730   78.9875   0.2782
4   0.6011   93.5552   0.4525

5 0.5210 62.5160 0.4234
6 0.5382 66.9169 0.5482
7 0.3932 46.2943 0.4961
8 0.4656 52.7928 0.2878
9 0.4257 48.5661 0.4662
10 0.4689 53.2292 0.2865
11 0.3224 44.1419 0.9310
12 0.3869 45.9547 0.2758
13 0.3660 45.0440 0.1547
14 0.3119 44.1205 0.4642
15 0.3119 44.1205 0.3490

$Best.nc
KL CH Hartigan CCC Scott Marriot TrCovW TraceW Friedman Rubin Cindex DB Silhouette
Number_clusters 4.0000 4.0000 3.000 5.0000 3.0000 3 3.00 3.0000 14.0000 5.0000 11.000 2.0000 2.000
Value_Index 3.3568 187.4822 59.481 3.5453 293.7961 2971502 28357.19 95.2098 2.1957 -0.1383 0.191 0.8006 0.504
Duda PseudoT2 Beale Ratkowsky Ball PtBiserial Frey McClain Dunn Hubert SDindex Dindex SDbw
Number_clusters 4.0000 4.0000 2.0000 4.0000 3.0000 2.0000 2.0000 2.000 2.0000 0 2.0000 0 15.0000
Value_Index 0.6582 73.2185 0.9756 0.3948 143.9043 0.6301 2.3784 0.123 0.0826 0 2.0966 0 0.2446

$Best.partition
OSR_69 OSR_137 OSR_186 OSR_388 OSR_389 OSR_390 OSR_489 OSR_490 OSR_491 OSR_498 OSR_499 OSR_500 OSR_502 OSR_508
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_520 OSR_521 OSR_522 OSR_523 OSR_524 OSR_525 OSR_538 OSR_539 OSR_541 OSR_542 OSR_546 OSR_547 OSR_548 OSR_551
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_634 OSR_635 OSR_636 OSR_639 OSR_749 OSR_831 OSR_834 OSR_836 OSR_837 OSR_838 OSR_839 OSR_841 OSR_842 OSR_843
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_844 OSR_846 OSR_847 OSR_849 OSR_850 OSR_851 OSR_852 OSR_853 OSR_854 OSR_855 OSR_856 OSR_857 OSR_858 OSR_859
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_860 OSR_862 OSR_863 OSR_864 OSR_865 OSR_866 OSR_867 OSR_870 OSR_871 OSR_872 OSR_873 OSR_874 OSR_875 OSR_876
2 1 1 1 1 2 1 1 1 1 1 1 1 1
OSR_877 OSR_878 OSR_880 OSR_884 OSR_886 OSR_887 OSR_888 OSR_889 OSR_890 OSR_891 OSR_892 OSR_893 OSR_894 OSR_895
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_896 OSR_898 OSR_899 OSR_900 OSR_901 OSR_902 OSR_903 OSR_904 OSR_924 OSR_925 OSR_947 OSR_960 OSR_962 OSR_969
1 1 2 1 1 1 1 1 1 1 1 1 1 1
OSR_970 OSR_971 OSR_972 OSR_973 OSR_974 OSR_975 OSR_976 OSR_977 OSR_978 OSR_979 OSR_980 OSR_981 OSR_982 OSR_983

1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_984 OSR_985 OSR_986 OSR_987 OSR_988 OSR_989 OSR_990 OSR_991
OSR_992 OSR_993 OSR_994 OSR_995 OSR_996 OSR_997
1 1 1 1 1 1 2 2 1 1 1 1 1 1
OSR_998 OSR_999 OSR_1000 OSR_1001 OSR_1002 OSR_1003 OSR_1004 OSR_1005
OSR_1006 OSR_1007 OSR_1008 OSR_1009 OSR_1010 OSR_1011
1 1 1 1 1 1 1 1 1 1 1 2 1 1
OSR_1012 OSR_1013 OSR_1014 OSR_1015 OSR_1016 OSR_1098 OSR_1099 OSR_1100
OSR_1101 OSR_1102 OSR_1103 OSR_1105 OSR_1106 OSR_1107
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1108 OSR_1109 OSR_1110 OSR_1111 OSR_1112 OSR_1113 OSR_1114 OSR_1115
OSR_1116 OSR_1118 OSR_1119 OSR_1123 OSR_1124 OSR_1126
1 1 1 1 1 1 1 1 1 1 1 2 2 2
OSR_1127 OSR_1128 OSR_1129 OSR_1130 OSR_1131 OSR_1133 OSR_1134 OSR_1136
OSR_1137 OSR_1138 OSR_1139 OSR_1350 OSR_1351 OSR_1352
2 2 2 2 2 2 2 2 2 2 2 2 2 2
OSR_1353 OSR_1354 OSR_1355 OSR_1356 OSR_1357 OSR_1358 OSR_1359 OSR_1360
OSR_1361 OSR_1362 OSR_1364 OSR_1365 OSR_1367 OSR_1368
2 2 2 2 2 1 1 1 1 1 1 1 1 1
OSR_1369 OSR_1370 OSR_1371 OSR_1372 OSR_1373 OSR_1374 OSR_1375 OSR_1376
OSR_1377 OSR_1378 OSR_1379 OSR_1380 OSR_1381 OSR_1382
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1383 OSR_1384 OSR_1385 OSR_1386 OSR_1387 OSR_1388 OSR_1389 OSR_1390
OSR_1391 OSR_1392 OSR_1393 OSR_1403 OSR_1404 OSR_1829
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1830 OSR_1831 OSR_1832 OSR_1833 OSR_1834 OSR_1835 OSR_1836 OSR_1837
OSR_1838 OSR_1839 OSR_1840 OSR_1841 OSR_1842 OSR_1843
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1844 OSR_1845 OSR_1846 OSR_1847 OSR_1848 OSR_1849 OSR_1850 OSR_1851
OSR_1852 OSR_1853 OSR_1854 OSR_1855 OSR_1856 OSR_1857
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1858 OSR_1859 OSR_1860 OSR_1861 OSR_1926 OSR_1927 OSR_1928 OSR_1929
OSR_1930 OSR_1931 OSR_1932 OSR_1933 OSR_1934 OSR_1935
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1936 OSR_1937 OSR_1938 OSR_1939 OSR_2034 OSR_2035 OSR_2036 OSR_2037
OSR_2038 OSR_2039 OSR_2040 OSR_2041 OSR_2042 OSR_2043
1 1 1 1 1 1 2 2 1 1 1 1 1 2
OSR_2044 OSR_2045 OSR_2046
1 2 1

NbClust(data = enamelclean, diss = NULL, distance = "euclidean", min.nc = 3, max.nc = 15, method = "ward.D2") #based on the dendrogram
*** : The Hubert index is a graphical method of determining the number of clusters.
In the plot of Hubert index, we seek a significant knee that corresponds to a significant increase of the value of the measure i.e the significant peak in Hubert
index second differences plot.

*** : The D index is a graphical method of determining the number of clusters.
In the plot of D index, we seek a significant knee (the significant peak in Dindex
second differences plot) that corresponds to a significant increase of the value of
the measure.

****
* Among all indices:
* 2 proposed 3 as the best number of clusters
* 13 proposed 4 as the best number of clusters
* 3 proposed 5 as the best number of clusters
* 1 proposed 11 as the best number of clusters
* 2 proposed 14 as the best number of clusters
* 2 proposed 15 as the best number of clusters

***** Conclusion *****

* According to the majority rule, the best number of clusters is 4

****
$All.index

	KL	CH	Hartigan	CCC	Scott	Marriot	TrCovW	TraceW	Friedman	Rubin	Cindex	DB	Silhouette
3	2.3717	187.1209	81.4100	1.5286	765.9459	9748395	21085.730	344.7945	6.4886	2.4507	0.2314	1.1375	0.3594
4	3.3568	187.4822	51.1928	3.4621	915.0431	10233040	10342.397	267.1273	7.4198	3.1633	0.2840	1.0506	0.3596
5	1.9959	178.5679	32.8307	3.5453	1051.5002	9872255	6720.973	225.7121	8.7511	3.7437	0.2582	1.1100	0.2963
6	0.9245	165.6928	26.7376	2.8183	1138.8970	10438999	4989.475	201.8718	10.0838	4.1858	0.2415	1.1403	0.2835
7	1.5251	155.2990	23.6211	2.1809	1228.1339	10365938	4138.681	184.1013	11.8076	4.5899	0.2246	1.2063	0.2863
8	2.6690	147.3444	21.6993	1.7118	1303.4290	10376332	3707.391	169.5874	13.5747	4.9827	0.2172	1.2359	0.2635
9	0.2879	141.2962	22.5864	1.3957	1353.0961	11018674	2910.180	157.1845	14.1669	5.3759	0.2090	1.2345	0.2328
10	0.9239	137.9541	20.7745	1.4021	1410.0089	11125139	2394.224	145.2142	14.8384	5.8190	0.2011	1.2323	0.2393

11 0.7104 135.1872 20.2968 1.4337 1478.1394 10581254 2066.628 134.9453
16.9373 6.2618 0.1910 1.1727 0.2452
12 1.0047 133.4209 18.9103 1.5727 1532.7282 10383450 1741.335 125.5748
17.7234 6.7291 0.2506 1.0775 0.2526
13 1.3902 131.9240 16.5999 1.7136 1592.9097 9851692 1467.747 117.3838
18.8410 7.1986 0.2430 1.0393 0.2581
14 0.8738 130.0564 16.0257 1.7587 1649.8063 9344718 1300.296 110.5850
21.0367 7.6412 0.2378 1.0248 0.2627
15 0.9170 128.6261 15.4746 1.8440 1702.4163 8907520 1112.950 104.3673
22.4241 8.0964 0.2422 1.0626 0.2587
Duda Pseudot2 Beale Ratkowsky Ball Ptbiserial Frey McClain Dunn Hubert
SDindex Dindex SDbw
3 0.5668 81.0137 1.2890 0.3769 114.9315 0.5455 0.3897 0.7318 0.0364 0.0029
2.2958 0.9776 0.7368
4 0.6582 73.2185 0.8778 0.3948 66.7818 0.5627 1.7598 0.8879 0.0500 0.0031
2.1626 0.8693 0.6697
5 0.6415 38.0022 0.9376 0.3730 45.1424 0.4598 0.3584 1.6421 0.0399 0.0033
2.6682 0.7854 0.6850
6 0.7037 32.8476 0.7079 0.3473 33.6453 0.4538 0.6614 1.8261 0.0399 0.0035
2.6120 0.7417 0.4981
7 0.6726 14.6007 0.8018 0.3263 26.3002 0.4234 0.0926 2.2640 0.0376 0.0037
2.7750 0.7081 0.4593
8 0.5678 35.0109 1.2682 0.3079 21.1984 0.4261 0.4879 2.2836 0.0376 0.0039
2.7531 0.6795 0.5777
9 0.6592 18.6134 0.8564 0.2946 17.4649 0.4141 0.1170 2.4840 0.0376 0.0039
2.9043 0.6435 0.5033
10 0.5673 35.8537 1.2716 0.2835 14.5214 0.4154 0.2356 2.5121 0.0376 0.0040
3.1031 0.6250 0.4827
11 0.9168 1.9052 0.1474 0.2718 12.2678 0.4108 -0.0535 2.6216 0.0376 0.0040
3.1537 0.6000 0.3866
12 0.5565 23.1146 1.3117 0.2630 10.4646 0.4133 0.2661 2.5984 0.0500 0.0041
2.8314 0.5891 0.2671
13 0.4771 28.4943 1.7966 0.2549 9.0295 0.4095 0.3732 2.6716 0.0500 0.0041
2.8114 0.5693 0.3196
14 0.6521 10.6721 0.8652 0.2465 7.8989 0.4045 0.1383 2.7536 0.0500 0.0041
2.8376 0.5503 0.2607
15 0.5919 13.7897 1.1179 0.2394 6.9578 0.4041 0.1975 2.7700 0.0522 0.0042
2.8099 0.5388 0.2446

$All.CriticalValues

	CritValue_Duda	CritValue_PseudoT2	Fvalue_Beale
3	0.5730	78.9875	0.2782
4	0.6011	93.5552	0.4525
5	0.5210	62.5160	0.4234
6	0.5382	66.9169	0.5482
7	0.3932	46.2943	0.4961
8	0.4656	52.7928	0.2878
9	0.4257	48.5661	0.4662
10	0.4689	53.2292	0.2865
11	0.3224	44.1419	0.9310

```
12       0.3869          45.9547     0.2758
13       0.3660          45.0440     0.1547
14       0.3119          44.1205     0.4642
15       0.3119          44.1205     0.3490

$Best.nc
              KL      CH Hartigan    CCC    Scott  Marriot   TrCovW TraceW Friedman   Rubin
Cindex     DB
Number_clusters 4.0000   4.0000   4.0000 5.0000   4.0000      5.0     4.00  4.000  14.0000
5.0000 11.000 14.0000
Value_Index     3.3568 187.4822  30.2172 3.5453 149.0972 927529.6 10743.33 36.252
2.1957 -0.1383  0.191  1.0248
           Silhouette   Duda PseudoT2 Beale Ratkowsky    Ball PtBiserial Frey McClain
Dunn Hubert SDindex
Number_clusters     4.0000 4.0000   4.0000 3.000    4.0000  4.0000     4.0000   2  3.0000
15.0000     0  4.0000
Value_Index       0.3596 0.6582  73.2185 1.289    0.3948 48.1497     0.5627   NA  0.7318
0.0522     0  2.1626
           Dindex   SDbw
Number_clusters     0 15.0000
Value_Index        0  0.2446

$Best.partition
 OSR_69  OSR_137  OSR_186  OSR_388  OSR_389  OSR_390  OSR_489  OSR_490
OSR_491  OSR_498  OSR_499  OSR_500
     1       1       1       1       2       1       2       2       1       1       2       2
 OSR_502  OSR_508  OSR_520  OSR_521  OSR_522  OSR_523  OSR_524  OSR_525
OSR_538  OSR_539  OSR_541  OSR_542
     1       2       2       2       2       2       2       2       2       2       1       1
 OSR_546  OSR_547  OSR_548  OSR_551  OSR_634  OSR_635  OSR_636  OSR_639
OSR_749  OSR_831  OSR_834  OSR_836
     1       2       1       1       1       1       1       1       2       2       2       1
 OSR_837  OSR_838  OSR_839  OSR_841  OSR_842  OSR_843  OSR_844  OSR_846
OSR_847  OSR_849  OSR_850  OSR_851
     2       2       2       2       2       1       1       1       2       2       2       2
 OSR_852  OSR_853  OSR_854  OSR_855  OSR_856  OSR_857  OSR_858  OSR_859
OSR_860  OSR_862  OSR_863  OSR_864
     2       1       2       2       2       1       1       2       3       2       2       4
 OSR_865  OSR_866  OSR_867  OSR_870  OSR_871  OSR_872  OSR_873  OSR_874
OSR_875  OSR_876  OSR_877  OSR_878
     2       3       1       2       2       2       2       1       4       4       1       2
 OSR_880  OSR_884  OSR_886  OSR_887  OSR_888  OSR_889  OSR_890  OSR_891
OSR_892  OSR_893  OSR_894  OSR_895
     1       1       1       1       1       4       1       4       4       1       1       1
 OSR_896  OSR_898  OSR_899  OSR_900  OSR_901  OSR_902  OSR_903  OSR_904
OSR_924  OSR_925  OSR_947  OSR_960
     1       1       3       1       2       2       1       1       2       2       2       2
 OSR_962  OSR_969  OSR_970  OSR_971  OSR_972  OSR_973  OSR_974  OSR_975
OSR_976  OSR_977  OSR_978  OSR_979
     2       1       2       2       1       1       1       2       2       2       2       1
```

OSR_980 OSR_981 OSR_982 OSR_983 OSR_984 OSR_985 OSR_986 OSR_987
OSR_988 OSR_989 OSR_990 OSR_991
2 2 2 2 2 2 2 2 2 2 3 3
OSR_992 OSR_993 OSR_994 OSR_995 OSR_996 OSR_997 OSR_998 OSR_999
OSR_1000 OSR_1001 OSR_1002 OSR_1003
2 2 2 2 2 2 2 2 2 2 2 2
OSR_1004 OSR_1005 OSR_1006 OSR_1007 OSR_1008 OSR_1009 OSR_1010 OSR_1011
OSR_1012 OSR_1013 OSR_1014 OSR_1015
2 2 2 1 2 3 1 2 2 1 2 2
OSR_1016 OSR_1098 OSR_1099 OSR_1100 OSR_1101 OSR_1102 OSR_1103 OSR_1105
OSR_1106 OSR_1107 OSR_1108 OSR_1109
2 2 2 2 2 2 2 2 1 2 1 2
OSR_1110 OSR_1111 OSR_1112 OSR_1113 OSR_1114 OSR_1115 OSR_1116 OSR_1118
OSR_1119 OSR_1123 OSR_1124 OSR_1126
2 1 2 2 1 1 2 1 2 3 3 3
OSR_1127 OSR_1128 OSR_1129 OSR_1130 OSR_1131 OSR_1133 OSR_1134 OSR_1136
OSR_1137 OSR_1138 OSR_1139 OSR_1350
3 3 3 3 3 3 3 3 3 3 3 3
OSR_1351 OSR_1352 OSR_1353 OSR_1354 OSR_1355 OSR_1356 OSR_1357 OSR_1358
OSR_1359 OSR_1360 OSR_1361 OSR_1362
3 3 3 3 3 3 3 2 2 2 2 1
OSR_1364 OSR_1365 OSR_1367 OSR_1368 OSR_1369 OSR_1370 OSR_1371 OSR_1372
OSR_1373 OSR_1374 OSR_1375 OSR_1376
2 2 2 2 2 2 2 2 2 2 2 2
OSR_1377 OSR_1378 OSR_1379 OSR_1380 OSR_1381 OSR_1382 OSR_1383 OSR_1384
OSR_1385 OSR_1386 OSR_1387 OSR_1388
2 2 2 2 2 2 2 4 2 2 2 2
OSR_1389 OSR_1390 OSR_1391 OSR_1392 OSR_1393 OSR_1403 OSR_1404 OSR_1829
OSR_1830 OSR_1831 OSR_1832 OSR_1833
1 2 2 2 2 2 1 4 4 2 4 2
OSR_1834 OSR_1835 OSR_1836 OSR_1837 OSR_1838 OSR_1839 OSR_1840 OSR_1841
OSR_1842 OSR_1843 OSR_1844 OSR_1845
4 2 2 4 4 4 4 2 4 4 4 4
OSR_1846 OSR_1847 OSR_1848 OSR_1849 OSR_1850 OSR_1851 OSR_1852 OSR_1853
OSR_1854 OSR_1855 OSR_1856 OSR_1857
4 4 4 4 4 4 4 4 4 4 4 4
OSR_1858 OSR_1859 OSR_1860 OSR_1861 OSR_1926 OSR_1927 OSR_1928 OSR_1929
OSR_1930 OSR_1931 OSR_1932 OSR_1933
4 4 2 4 4 1 1 2 4 2 1 2
OSR_1934 OSR_1935 OSR_1936 OSR_1937 OSR_1938 OSR_1939 OSR_2034 OSR_2035
OSR_2036 OSR_2037 OSR_2038 OSR_2039
4 1 2 1 2 4 2 1 3 3 2 1
OSR_2040 OSR_2041 OSR_2042 OSR_2043 OSR_2044 OSR_2045 OSR_2046
1 1 1 3 1 3 1

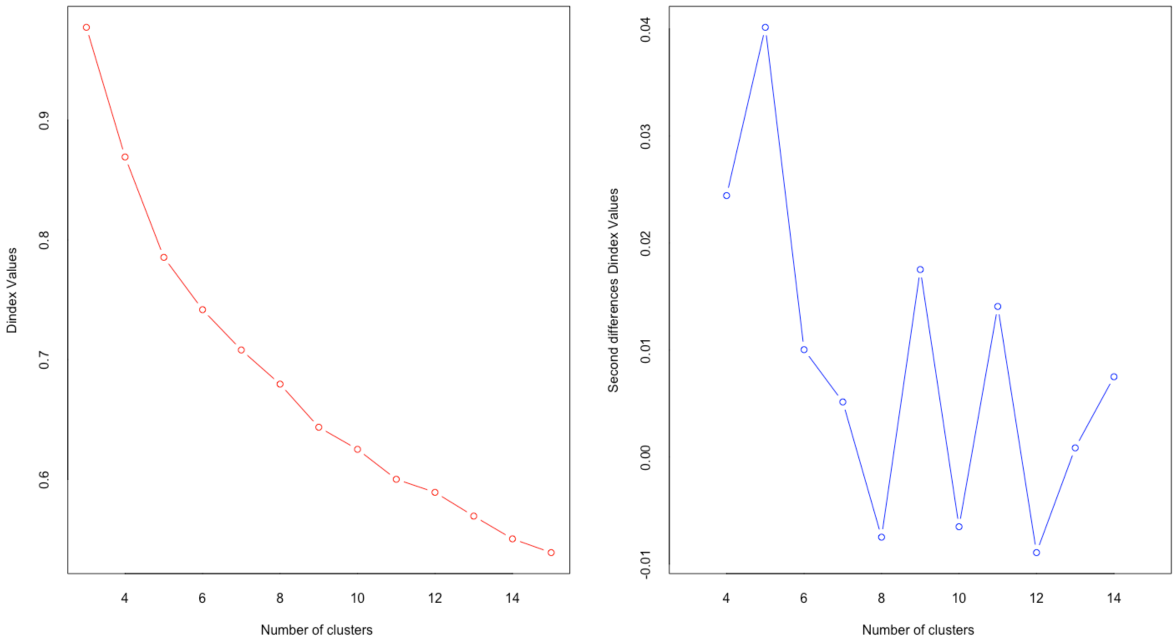


Figure F-1: Hierarchical clustering of enamel δ^{18}O, δ^{13}C and $^{87/86}$Sr data D-index outputs for optimal clusters.

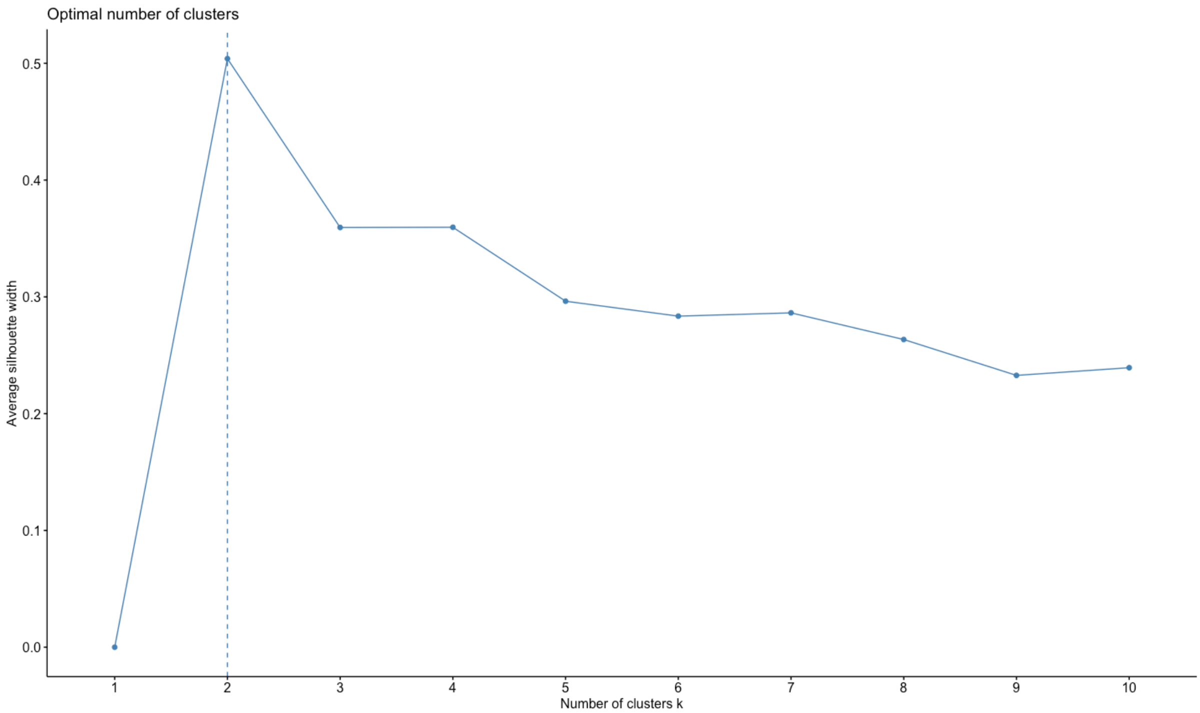


Figure F-2: Silhouette method for optimal number of hierarchical clusters for enamel δ δ^{18}O, δ^{13}C and $^{87/86}$Sr.

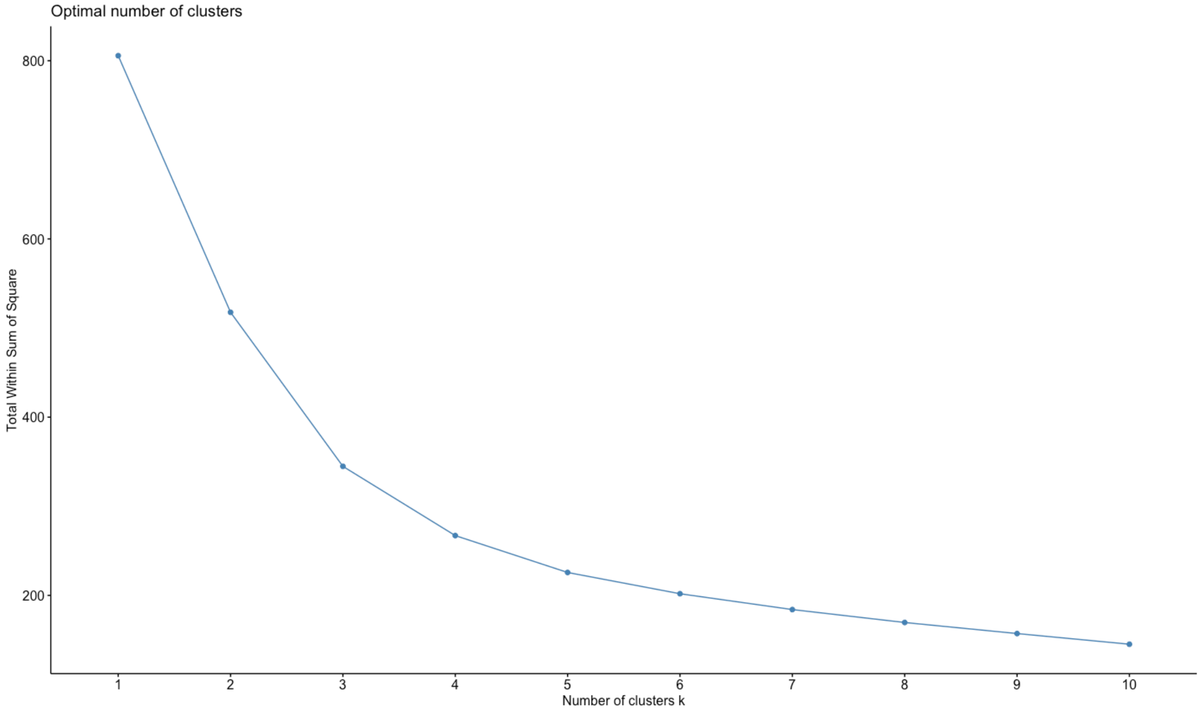


Figure F-3: Elbow method for optimal number of hierarchical clusters for enamel δ $\delta^{18}O$, $\delta^{13}C$ and $^{87/86}Sr$.

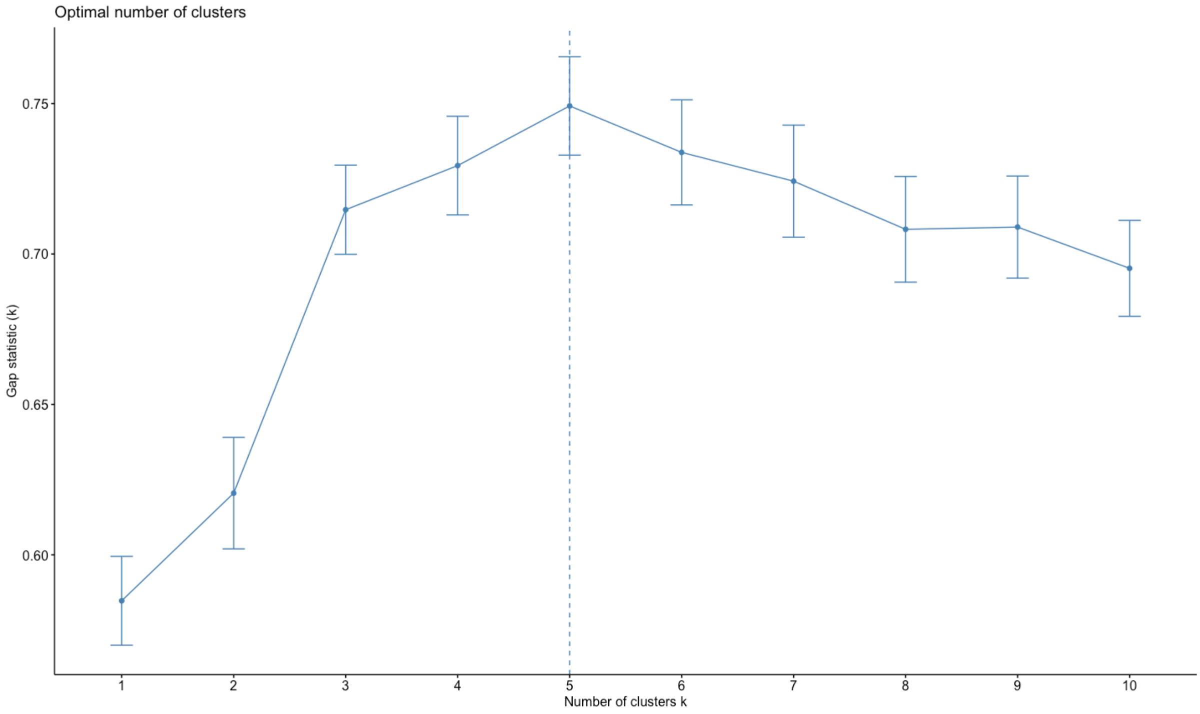


Figure F-4: Gap statistic method for optimal number of hierarchical clusters for enamel δ $\delta^{18}O$, $\delta^{13}C$ and $^{87/86}Sr$.

F.ii Enamel Combination 2 (O, Sr)

NbClust(data = OSrClean, diss = NULL, distance = "euclidean", min.nc = 2, max.nc = 15, method = "ward.D2")

*** : The Hubert index is a graphical method of determining the number of clusters.
In the plot of Hubert index, we seek a significant knee that corresponds to a significant increase of the value of the measure i.e the significant peak in
Hubert
index second differences plot.

*** : The D index is a graphical method of determining the number of clusters.
In the plot of D index, we seek a significant knee (the significant peak in Dindex
second differences plot) that corresponds to a significant increase of the value of
the measure.

****
* Among all indices:
* 1 proposed 2 as the best number of clusters
* 14 proposed 3 as the best number of clusters
* 2 proposed 4 as the best number of clusters
* 4 proposed 5 as the best number of clusters
* 1 proposed 13 as the best number of clusters
* 1 proposed 14 as the best number of clusters

***** Conclusion *****

* According to the majority rule, the best number of clusters is 3

****
$All.index
KL CH Hartigan CCC Scott Marriot TrCovW TraceW Friedman Rubin
Cindex DB Silhouette Duda
2 0.6536 507.7338 613.7518 -4.7030 816.6411 380224.8 96280.248 662.6815
2.0354 1.7532 0.1412 1.1676 0.5028 0.3512
3 33.4429 784.4451 237.8147 1.8993 1625.6897 267092.3 34375.885 351.4350
4.8536 3.3060 0.1969 0.7610 0.5261 0.5086
4 0.1488 780.8281 220.1797 1.8249 2013.3324 271836.0 17434.066 261.5500
6.9552 4.4421 0.1615 0.9038 0.3820 0.5653
5 0.9973 826.0706 94.7879 3.3955 2432.2636 232457.5 6888.577 198.3484
10.2932 5.8575 0.1628 0.9774 0.3955 0.4620
6 3.1917 769.4816 101.9009 1.4067 2592.5595 265790.6 5312.333 174.3916
11.6557 6.6622 0.1557 0.9206 0.3747 0.5432
7 4.6266 751.9617 101.0295 0.7552 2808.7615 265052.6 4281.259 151.9227
14.2071 7.6475 0.1406 0.8456 0.3920 0.5565
8 3.8333 752.5234 85.1721 0.7471 2990.9868 266346.1 2739.739 132.4701
16.3710 8.7705 0.1234 0.9140 0.3580 0.6119
9 0.3050 749.6452 73.9563 0.6116 3137.3350 273086.8 2734.218 117.8584
18.2356 9.8579 0.1203 0.9377 0.3526 0.4381
10 0.2375 745.3187 59.1857 0.4216 3265.0879 280533.6 2374.543 106.3888
20.0019 10.9206 0.1098 0.9634 0.3291 0.5946
11 1.6171 733.5906 56.5211 -0.0391 3388.0182 284415.4 1793.312 97.9276
22.1783 11.8642 0.1071 0.9700 0.3350 0.6767
12 2.4133 726.0838 59.2500 -0.3505 3506.1374 285574.4 1578.622 90.4532
24.5146 12.8446 0.1233 1.0553 0.3304 0.4936
13 0.4998 727.1866 57.1253 -0.3473 3614.6665 286698.5 1580.466 83.2328
26.5602 13.9588 0.1166 1.0570 0.3406 0.5875

14 0.6926 730.7951 42.0140 -0.2537 3715.6492 287536.1 1411.140 76.7999
28.4453 15.1280 0.1060 1.0534 0.3509 0.5347
15 6.6945 722.3998 44.3503 -0.6002 3802.0713 291484.2 1101.303 72.3371
30.4514 16.0614 0.1444 1.0260 0.3517 0.5106
Pseudot2 Beale Ratkowsky Ball Ptbiserial Frey McClain Dunn Hubert SDindex
Dindex SDbw
2 389.7461 1.8384 0.4418 331.3408 0.5665 -0.6360 0.3061 0.0144 0.0014
7.3089 0.7490 1.4834
3 463.6838 0.9640 0.4810 117.1450 0.6521 3.1663 0.2850 0.0230 0.0018
3.7959 0.6013 0.5836
4 138.4265 0.7648 0.4392 65.3875 0.4796 0.1046 0.7964 0.0099 0.0019 4.5308
0.4922 0.6261
5 149.0403 1.1554 0.4068 39.6697 0.4994 0.6123 0.7870 0.0116 0.0020 4.3789
0.4382 0.5219
6 203.5052 0.8375 0.3760 29.0653 0.4952 0.4849 0.8142 0.0116 0.0021 4.1363
0.4088 0.4671
7 188.0912 0.7936 0.3521 21.7032 0.4897 1.1967 0.8510 0.0116 0.0021 4.1230
0.3855 0.4271
8 31.7101 0.6218 0.3326 16.5588 0.4435 0.0494 1.0670 0.0116 0.0022 5.2910
0.3493 0.3685
9 274.5285 1.2769 0.3158 13.0954 0.4453 1.8162 1.0538 0.0116 0.0022 5.0190
0.3372 0.2944
10 26.5878 0.6647 0.3012 10.6389 0.3861 0.1093 1.4243 0.0116 0.0023 6.3982
0.3071 0.2606
11 13.8564 0.4619 0.2884 8.9025 0.3867 0.0517 1.4101 0.0116 0.0023 6.3182
0.2979 0.2270
12 94.3985 1.0150 0.2770 7.5378 0.3874 0.5249 1.3963 0.0136 0.0023 5.9255
0.2921 0.2141
13 107.4147 0.6975 0.2671 6.4025 0.3792 1.0139 1.4374 0.0136 0.0023 6.0611
0.2779 0.2019
14 14.7924 0.8218 0.2582 5.4857 0.3454 0.0074 1.6972 0.0136 0.0023 6.6834
0.2632 0.2166
15 19.1725 0.9130 0.2499 4.8225 0.3457 0.0772 1.6882 0.0187 0.0023 7.3670
0.2597 0.2043

$All.CriticalValues

	CritValue_Duda	CritValue_PseudoT2	Fvalue_Beale
2	0.5126	200.6259	0.1603
3	0.5693	363.1610	0.3817
4	0.4988	180.8900	0.4662
5	0.4653	147.1195	0.3166
6	0.5237	220.0901	0.4334
7	0.5217	216.3426	0.4528
8	0.3395	97.2875	0.5391
9	0.5138	202.5209	0.2800
10	0.2963	92.6281	0.5173
11	0.2385	92.6108	0.6324
12	0.4272	123.3764	0.3644
13	0.4835	163.4595	0.4986
14	0.1155	130.1288	0.4482

15 0.1556 108.5678 0.4095

$Best.nc
KL CH Hartigan CCC Scott Marriot TrCovW TraceW Friedman
Rubin Cindex DB Silhouette
Number_clusters 3.0000 5.0000 3.0000 5.0000 3.0000 3.0 3.00 3.0000
5.000 5.0000 14.000 3.000 3.0000
Value_Index 33.4429 826.0706 375.9371 3.3955 809.0486 117876.3 61904.36
221.3615 3.338 -0.6108 0.106 0.761 0.5261
Duda PseudoT2 Beale Ratkowsky Ball PtBiserial Frey McClain Dunn
Hubert SDindex Dindex SDbw
Number_clusters 4.0000 4.0000 2.0000 3.000 3.0000 3.0000 1 3.000 3.000
0 3.0000 0 13.0000
Value_Index 0.5653 138.4265 1.8384 0.481 214.1958 0.6521 NA 0.285 0.023
0 3.7959 0 0.2019

$Best.partition
OSR_69 OSR_137 OSR_186 OSR_199 OSR_200 OSR_201 OSR_202 OSR_210
OSR_211 OSR_212 OSR_213 OSR_214 OSR_215 OSR_216
1 1 1 2 2 2 2 2 2 2 2 2 2 2
OSR_217 OSR_218 OSR_219 OSR_220 OSR_221 OSR_222 OSR_223 OSR_224
OSR_225 OSR_226 OSR_227 OSR_228 OSR_283 OSR_284
2 2 2 2 2 2 2 2 2 2 2 2 1 2
OSR_285 OSR_286 OSR_287 OSR_288 OSR_289 OSR_290 OSR_291 OSR_292
OSR_293 OSR_294 OSR_295 OSR_296 OSR_297 OSR_298
2 2 2 2 2 2 2 2 2 1 2 2 2 2
OSR_300 OSR_301 OSR_302 OSR_303 OSR_304 OSR_305 OSR_306 OSR_307
OSR_368 OSR_369 OSR_370 OSR_371 OSR_372 OSR_373
2 2 2 2 2 2 2 1 2 2 2 2 2 2
OSR_374 OSR_375 OSR_376 OSR_377 OSR_378 OSR_379 OSR_382 OSR_383
OSR_388 OSR_389 OSR_390 OSR_391 OSR_392 OSR_393
2 2 2 2 1 2 2 2 1 1 1 2 2 2
OSR_394 OSR_395 OSR_396 OSR_397 OSR_398 OSR_399 OSR_400 OSR_401
OSR_402 OSR_403 OSR_404 OSR_405 OSR_406 OSR_407
2 2 2 2 2 2 2 2 2 2 2 2 2 2
OSR_408 OSR_409 OSR_410 OSR_411 OSR_412 OSR_413 OSR_414 OSR_415
OSR_416 OSR_417 OSR_418 OSR_419 OSR_420 OSR_421
2 2 2 2 2 1 2 2 2 2 2 2 2 2
OSR_425 OSR_426 OSR_427 OSR_428 OSR_429 OSR_430 OSR_431 OSR_433
OSR_437 OSR_438 OSR_442 OSR_443 OSR_444 OSR_445
1 2 2 2 2 2 2 2 2 2 2 2 1 2
OSR_446 OSR_448 OSR_450 OSR_451 OSR_452 OSR_453 OSR_454 OSR_455
OSR_456 OSR_457 OSR_458 OSR_459 OSR_460 OSR_461
2 1 2 1 1 2 2 2 2 2 1 2 1 2
OSR_462 OSR_463 OSR_464 OSR_465 OSR_466 OSR_467 OSR_474 OSR_475
OSR_476 OSR_477 OSR_478 OSR_479 OSR_480 OSR_481
2 2 2 2 2 1 2 2 2 2 2 2 2 2
OSR_482 OSR_483 OSR_484 OSR_485 OSR_486 OSR_487 OSR_488 OSR_489
OSR_490 OSR_491 OSR_498 OSR_499 OSR_500 OSR_502
2 2 2 2 2 2 2 2 2 1 2 2 2 1

```
 OSR_508  OSR_512  OSR_513  OSR_514  OSR_515  OSR_516  OSR_517  OSR_518 
OSR_519  OSR_520  OSR_521  OSR_522  OSR_523  OSR_524 
       2        2        2        2        2        2        2        2        2        2        2        2        2        2 
 OSR_525  OSR_531  OSR_532  OSR_533  OSR_534  OSR_535  OSR_536  OSR_537 
OSR_538  OSR_539  OSR_541  OSR_542  OSR_546  OSR_547 
       2        2        2        2        2        2        2        2        2        2        1        1        1        2 
 OSR_548  OSR_551  OSR_553  OSR_554  OSR_555  OSR_556  OSR_557  OSR_558 
OSR_559  OSR_560  OSR_561  OSR_562  OSR_563  OSR_564 
       1        1        2        2        2        2        2        2        2        2        2        2        2        2 
 OSR_565  OSR_566  OSR_567  OSR_568  OSR_569  OSR_570  OSR_571  OSR_572 
OSR_573  OSR_574  OSR_575  OSR_576  OSR_577  OSR_578 
       2        2        2        2        2        2        2        2        2        2        2        2        2        2 
 OSR_579  OSR_580  OSR_583  OSR_584  OSR_585  OSR_586  OSR_587  OSR_611 
OSR_634  OSR_635  OSR_636  OSR_639  OSR_640  OSR_641 
       2        2        2        2        1        2        2        2        1        2        1        1        2        2 
 OSR_642  OSR_643  OSR_644  OSR_645  OSR_646  OSR_660  OSR_661  OSR_663 
OSR_664  OSR_665  OSR_667  OSR_668  OSR_669  OSR_670 
       2        2        2        2        2        2        2        1        2        2        2        2        2        2 
 OSR_671  OSR_672  OSR_673  OSR_674  OSR_675  OSR_676  OSR_677  OSR_678 
OSR_679  OSR_680  OSR_681  OSR_682  OSR_683  OSR_684 
       2        2        2        2        2        2        2        2        2        2        2        2        2        2 
 OSR_685  OSR_686  OSR_687  OSR_688  OSR_692  OSR_693  OSR_694  OSR_695 
OSR_696  OSR_697  OSR_698  OSR_699  OSR_700  OSR_701 
       2        2        2        2        2        2        2        2        2        2        2        2        2        2 
 OSR_702  OSR_703  OSR_704  OSR_738  OSR_739  OSR_740  OSR_743  OSR_744 
OSR_745  OSR_747  OSR_749  OSR_750  OSR_751  OSR_752 
       2        2        2        1        2        1        2        1        1        2        1        1        1        1 
 OSR_753  OSR_754  OSR_755  OSR_756  OSR_757  OSR_758  OSR_759  OSR_760 
OSR_761  OSR_762  OSR_763  OSR_764  OSR_778  OSR_779 
       1        1        1        1        1        1        1        2        2        2        2        2        2        2 
 OSR_780  OSR_781  OSR_782  OSR_783  OSR_788  OSR_790  OSR_791  OSR_792 
OSR_793  OSR_794  OSR_795  OSR_796  OSR_802  OSR_803 
       2        2        2        2        2        2        2        1        2        2        2        2        2        2 
 OSR_804  OSR_805  OSR_806  OSR_808  OSR_809  OSR_810  OSR_826  OSR_827 
OSR_828  OSR_829  OSR_830  OSR_831  OSR_834  OSR_836 
       2        2        2        2        2        2        2        2        2        2        2        2        2        1 
 OSR_837  OSR_838  OSR_839  OSR_841  OSR_842  OSR_843  OSR_844  OSR_846 
OSR_847  OSR_849  OSR_850  OSR_851  OSR_852  OSR_853 
       2        2        2        2        2        1        1        1        2        2        2        2        2        1 
 OSR_854  OSR_855  OSR_856  OSR_857  OSR_858  OSR_859  OSR_860  OSR_862 
OSR_863  OSR_864  OSR_865  OSR_866  OSR_867  OSR_870 
       2        2        2        1        1        2        1        2        2        1        2        1        1        2 
 OSR_871  OSR_872  OSR_873  OSR_874  OSR_875  OSR_876  OSR_877  OSR_878 
OSR_880  OSR_884  OSR_886  OSR_887  OSR_888  OSR_889 
       2        2        2        1        1        1        1        2        1        1        1        1        1        1 
 OSR_890  OSR_891  OSR_892  OSR_893  OSR_894  OSR_895  OSR_896  OSR_898 
OSR_899  OSR_900  OSR_901  OSR_902  OSR_903  OSR_904 
       1        1        1        1        1        1        1        1        3        1        2        2        1        1 
 OSR_924  OSR_925  OSR_947  OSR_960  OSR_962  OSR_969  OSR_970  OSR_971 
OSR_972  OSR_973  OSR_974  OSR_975  OSR_976  OSR_977 
```

2 2 2 2 2 1 2 2 1 1 1 2 2 2
OSR_978 OSR_979 OSR_980 OSR_981 OSR_982 OSR_983 OSR_984 OSR_985
OSR_986 OSR_987 OSR_988 OSR_989 OSR_990 OSR_991
2 1 2 2 2 2 2 2 1 2 2 2 1 3
OSR_992 OSR_993 OSR_994 OSR_995 OSR_996 OSR_997 OSR_998 OSR_999
OSR_1000 OSR_1001 OSR_1002 OSR_1003 OSR_1004 OSR_1005
2 2 1 2 2 2 2 2 2 2 2 2 2 2
OSR_1006 OSR_1007 OSR_1008 OSR_1009 OSR_1010 OSR_1011 OSR_1012 OSR_1013
OSR_1014 OSR_1015 OSR_1016 OSR_1098 OSR_1099 OSR_1100
2 1 2 3 1 2 2 1 2 2 1 2 2 2
OSR_1101 OSR_1102 OSR_1103 OSR_1105 OSR_1106 OSR_1107 OSR_1108 OSR_1109
OSR_1110 OSR_1111 OSR_1112 OSR_1113 OSR_1114 OSR_1115
2 2 2 2 1 2 1 2 2 1 2 2 1 1
OSR_1116 OSR_1118 OSR_1119 OSR_1123 OSR_1124 OSR_1126 OSR_1127 OSR_1128
OSR_1129 OSR_1130 OSR_1131 OSR_1133 OSR_1134 OSR_1136
1 1 2 1 1 3 3 3 3 3 3 3 3 3
OSR_1137 OSR_1138 OSR_1139 OSR_1220 OSR_1221 OSR_1222 OSR_1223 OSR_1224
OSR_1226 OSR_1227 OSR_1228 OSR_1229 OSR_1230 OSR_1231
3 3 3 2 3 2 1 1 1 3 1 2 3 2
OSR_1232 OSR_1233 OSR_1234 OSR_1235 OSR_1236 OSR_1237 OSR_1238 OSR_1239
OSR_1240 OSR_1241 OSR_1242 OSR_1244 OSR_1245 OSR_1246
1 1 1 1 1 1 1 3 1 1 3 2 1 3
OSR_1247 OSR_1248 OSR_1249 OSR_1250 OSR_1251 OSR_1252 OSR_1253 OSR_1254
OSR_1255 OSR_1256 OSR_1257 OSR_1342 OSR_1343 OSR_1344
1 2 2 2 2 3 2 1 1 1 1 2 2 1
OSR_1345 OSR_1346 OSR_1347 OSR_1348 OSR_1349 OSR_1350 OSR_1351 OSR_1352
OSR_1353 OSR_1354 OSR_1355 OSR_1356 OSR_1357 OSR_1358
2 2 2 1 2 3 3 1 3 3 3 3 3 2
OSR_1359 OSR_1360 OSR_1361 OSR_1362 OSR_1364 OSR_1365 OSR_1367 OSR_1368
OSR_1369 OSR_1370 OSR_1371 OSR_1372 OSR_1373 OSR_1374
2 2 2 1 2 2 2 2 2 2 2 2 2 2
OSR_1375 OSR_1376 OSR_1377 OSR_1378 OSR_1379 OSR_1380 OSR_1381 OSR_1382
OSR_1383 OSR_1384 OSR_1385 OSR_1386 OSR_1387 OSR_1388
2 2 2 2 2 2 2 2 1 1 2 2 2 2
OSR_1389 OSR_1390 OSR_1391 OSR_1392 OSR_1393 OSR_1394 OSR_1403 OSR_1404
OSR_1829 OSR_1830 OSR_1831 OSR_1832 OSR_1833 OSR_1834
1 2 2 2 2 2 2 1 1 1 2 1 2 1
OSR_1835 OSR_1836 OSR_1837 OSR_1838 OSR_1839 OSR_1840 OSR_1841 OSR_1842
OSR_1843 OSR_1844 OSR_1845 OSR_1846 OSR_1847 OSR_1848
2 2 1 1 1 2 2 1 1 1 1 1 1 1
OSR_1849 OSR_1850 OSR_1851 OSR_1852 OSR_1853 OSR_1854 OSR_1855 OSR_1856
OSR_1857 OSR_1858 OSR_1859 OSR_1860 OSR_1861 OSR_1897
1 1 1 1 1 1 1 1 1 1 1 2 1 1
OSR_1898 OSR_1899 OSR_1900 OSR_1901 OSR_1902 OSR_1903 OSR_1904 OSR_1905
OSR_1906 OSR_1907 OSR_1908 OSR_1909 OSR_1910 OSR_1911
2 2 2 1 2 2 2 2 2 2 2 2 2 1
OSR_1912 OSR_1913 OSR_1914 OSR_1915 OSR_1916 OSR_1917 OSR_1918 OSR_1919
OSR_1926 OSR_1927 OSR_1928 OSR_1929 OSR_1930 OSR_1931
2 2 2 2 2 2 2 2 1 1 1 2 1 2

```
OSR_1932 OSR_1933 OSR_1934 OSR_1935 OSR_1936 OSR_1937 OSR_1938 OSR_1939
OSR_1940 OSR_1941 OSR_1942 OSR_1943 OSR_1944 OSR_1945
       1        2        1        1        2        1        2        1        1        2        1        2        2        2
OSR_1946 OSR_1947 OSR_1948 OSR_1949 OSR_1950 OSR_1951 OSR_1952 OSR_1953
OSR_1954 OSR_1955 OSR_1956 OSR_1957 OSR_1958 OSR_1959
       2        1        1        2        1        2        2        1        2        2        2        2        2        2
OSR_1960 OSR_1961 OSR_1962 OSR_1963 OSR_1964 OSR_1965 OSR_1966 OSR_1967
OSR_1968 OSR_1969 OSR_1970 OSR_1971 OSR_1972 OSR_1973
       2        2        2        2        1        2        2        2        2        2        2        2        2        2
OSR_1974 OSR_1975 OSR_1976 OSR_1977 OSR_1978 OSR_1979 OSR_1980 OSR_1981
OSR_1982 OSR_1983 OSR_1984 OSR_1985 OSR_1986 OSR_1987
       2        2        2        2        2        2        2        2        2        1        2        2        2        2
OSR_1988 OSR_1989 OSR_1990 OSR_1991 OSR_1992 OSR_1993 OSR_1994 OSR_1995
OSR_1996 OSR_1997 OSR_2034 OSR_2035 OSR_2036 OSR_2037
       2        2        2        2        2        2        2        2        2        2        2        1        3        3
OSR_2038 OSR_2039 OSR_2040 OSR_2041 OSR_2042 OSR_2043 OSR_2044 OSR_2045
OSR_2046
       2        1        1        1        1        1        1        1        1
```

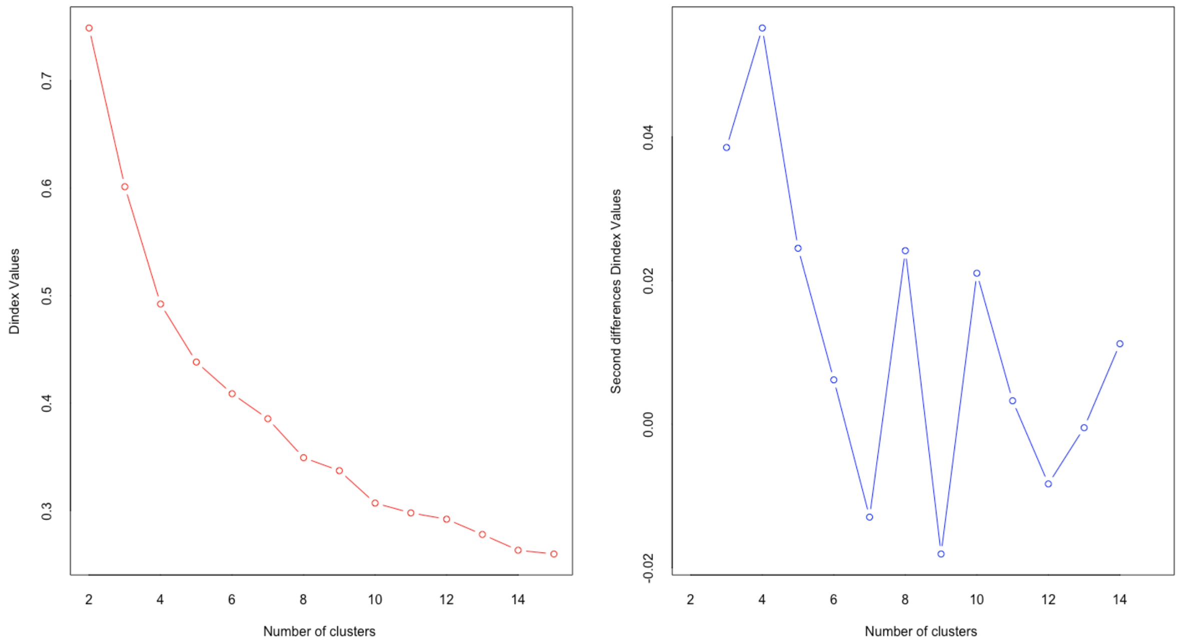


Figure F-5: Hierarchical clustering of enamel $\delta^{18}O$ and $^{87/86}Sr$ data D-index outputs for optimal clusters.

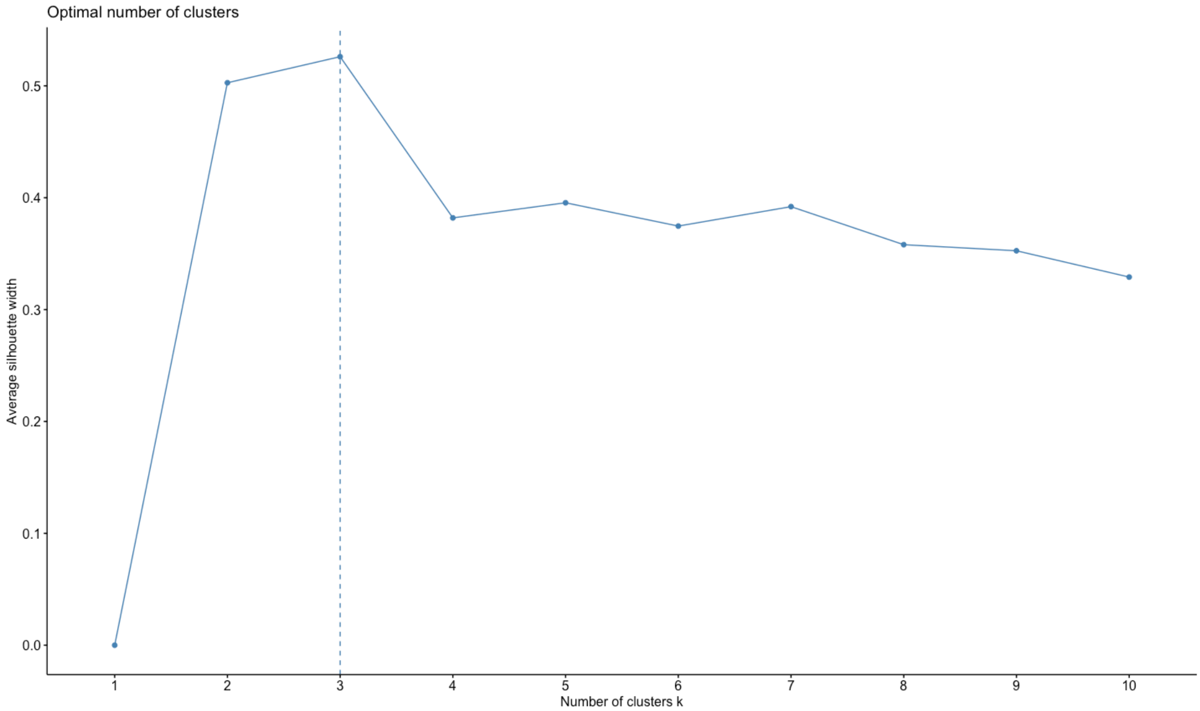


Figure F-6: Silhouette method for optimal number of hierarchical clusters for enamel $\delta^{18}O$ and $^{87/86}Sr$.

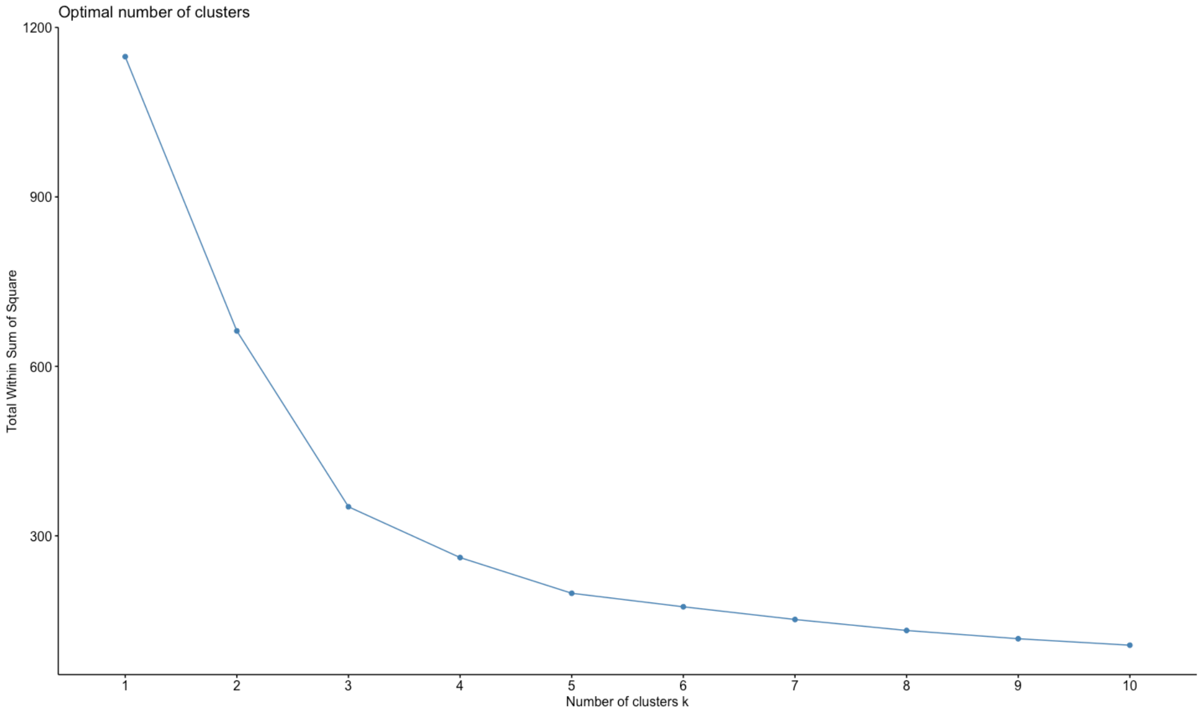


Figure F-7: Elbow method for optimal number of hierarchical clusters for enamel $\delta^{18}O$ and $^{87/86}Sr$.

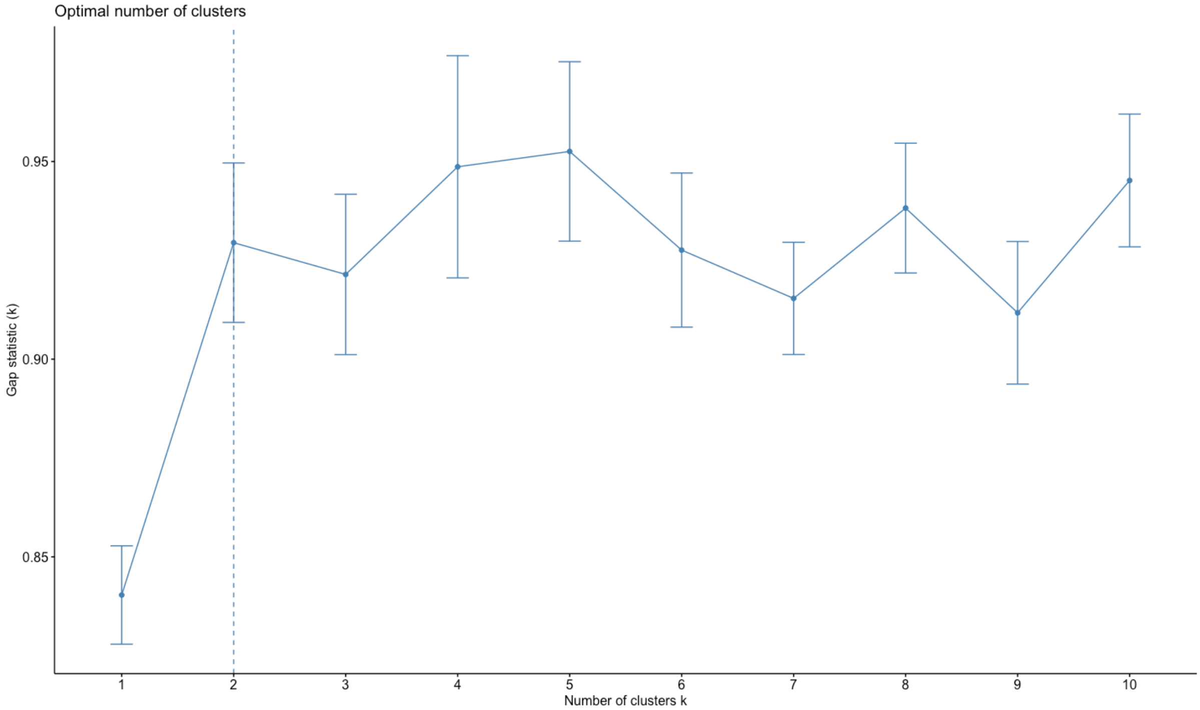


Figure F-8: Gap statistic method for optimal number of hierarchical clusters for enamel δ[18]O and [87/86]Sr.

F.iii Enamel Combination 3 (O, C)

NbClust(data = carbclean, diss = NULL, distance = "euclidean", min.nc = 2, max.nc = 15, method = "ward.D2")

*** : The Hubert index is a graphical method of determining the number of clusters.
In the plot of Hubert index, we seek a significant knee that corresponds to a significant increase of the value of the measure i.e the significant peak in Hubert
index second differences plot.

*** : The D index is a graphical method of determining the number of clusters.
In the plot of D index, we seek a significant knee (the significant peak in Dindex
second differences plot) that corresponds to a significant increase of the value of
the measure.

****

* Among all indices:
* 12 proposed 2 as the best number of clusters
* 9 proposed 3 as the best number of clusters
* 1 proposed 8 as the best number of clusters
* 1 proposed 12 as the best number of clusters
* 1 proposed 15 as the best number of clusters

***** Conclusion *****

* According to the majority rule, the best number of clusters is 2

```
******************************************************************
$All.index
     KL      CH Hartigan     CCC     Scott  Marriot     TrCovW   TraceW Friedman   Rubin
Cindex    DB Silhouette   Duda
2  73.0541 431.9653 289.4624 -1.6821  770.9514 403185.9 123372.158 673.6022
2.2257  1.9510 0.2286 0.7704     0.5675 0.6122
3   0.0299 467.3302 150.5988 -3.7781 1201.4617 434047.0  31487.416 449.8605
4.0060  2.9213 0.2129 1.1092     0.3264 0.5278
4   1.7847 441.7481 123.0981 -5.3435 1449.6004 504527.2  31395.251 357.2572
5.3540  3.6785 0.1898 1.0311     0.3067 0.6020
5   0.6017 431.6569  82.5831 -6.0410 1679.8066 531509.0  28429.271 294.7088
7.0741  4.4593 0.1629 1.0573     0.2991 0.6192
6   1.4584 410.3861  74.9290 -7.3300 1837.1785 584578.4  20313.028 257.9213
8.2785  5.0953 0.1567 1.1133     0.2869 0.5606
7   2.0772 398.1203  72.5035 -8.1340 1978.3564 624811.1  12864.920 228.3227
9.5716  5.7558 0.1465 1.0485     0.2994 0.5759
8   0.7261 393.7996  58.8412 -8.4787 2122.4310 637662.4   7834.218 202.8352
11.1666  6.4791 0.1363 1.0589     0.2909 0.6432
9   4.3079 386.4576  60.8914 -8.9975 2223.6227 678647.3   7635.233 184.0351
12.2861  7.1409 0.1829 0.9954     0.2950 0.5939
10  2.1197 385.9890  56.0056 -9.1029 2335.0868 692258.4   6792.642 166.4124
13.7903  7.8972 0.1695 1.0439     0.2927 0.4137
11  0.3647 386.2117  48.3285 -9.1612 2448.1772 690165.8   6695.945 151.6188
15.5255  8.6677 0.1638 0.9962     0.3014 0.6233
12  3.5649 384.4359  46.6222 -9.3362 2557.1150 681582.5   6671.020 139.8255
17.4902  9.3987 0.2222 1.0245     0.2973 0.6134
13  1.4100 384.3348  44.6591 -9.4067 2638.1572 696266.0   5062.503 129.2876
18.7540 10.1648 0.2095 1.0136     0.2867 0.6328
14  1.4949 385.2773  41.2036 -9.4112 2720.2529 701606.6   3821.019 119.9093
20.1517 10.9598 0.1970 1.0886     0.2864 0.6114
15  0.1041 385.8837  42.6422 -9.4340 2804.8465 696805.7   2938.700 111.8257
21.9663 11.7521 0.2223 1.0465     0.2879 0.3917
  Pseudot2  Beale Ratkowsky     Ball Ptbiserial    Frey McClain   Dunn Hubert SDindex
Dindex   SDbw
2  328.0795 0.6321    0.4503 336.8011     0.6754  3.9697  0.0992 0.0402 0.0020
3.3122 0.9365 0.8643
3  232.6520 0.8914    0.4534 149.9535     0.4793  0.9610  0.7099 0.0110 0.0018
3.5349 0.7584 0.9494
4  169.2246 0.6585    0.4170  89.3143     0.4517  0.7657  1.0355 0.0110 0.0018  3.3885
0.6690 1.0160
5   38.1342 0.6053    0.3870  58.9418     0.4095  0.0051  1.5656 0.0110 0.0020  3.5960
0.5960 0.8889
6   97.1897 0.7775    0.3606  42.9869     0.4164  0.2427  1.5583 0.0110 0.0022  3.4500
0.5613 0.6653
7   89.8542 0.7305    0.3392  32.6175     0.4163  0.4501  1.6290 0.0110 0.0023  3.7875
0.5303 0.5817
8   21.0783 0.5405    0.3216  25.3544     0.4049 -0.0843  1.7923 0.0110 0.0024  3.8665
0.4980 0.4832
```

```
9   92.9934 0.6788    0.3061  20.4483     0.4073  0.6537  1.7771 0.0150 0.0024  3.4123
0.4883 0.4065
10  87.8715 1.3948    0.2929  16.6412     0.3829  0.1643  2.0770 0.0150 0.0024  4.1852
0.4567 0.4120
11  21.1523 0.5876    0.2814  13.7835     0.3827  0.0865  2.0904 0.0150 0.0024  4.2752
0.4344 0.3706
12  81.9230 0.6254    0.2709  11.6521     0.3835  0.5999  2.0845 0.0208 0.0025  4.0132
0.4247 0.3804
13  55.1281 0.5743    0.2616   9.9452     0.3653  0.4953  2.3222 0.0208 0.0025  4.1165
0.4040 0.3559
14  13.3483 0.6067    0.2532   8.5650     0.3494  0.0630  2.5469 0.0208 0.0026  4.5988
0.3858 0.3083
15  88.5353 1.5265    0.2456   7.4550     0.3498  0.1660  2.5375 0.0237 0.0026  4.3877
0.3766 0.2749

$All.CriticalValues
  CritValue_Duda CritValue_PseudoT2 Fvalue_Beale
2         0.5735          385.2710       0.5317
3         0.5292          231.2790       0.4107
4         0.5281          228.7993       0.5181
5         0.3732          104.1223       0.5475
6         0.4618          144.4891       0.4607
7         0.4601          143.1725       0.4827
8         0.2915           92.3595       0.5847
9         0.4716          152.3680       0.5081
10        0.3732          104.1223       0.2517
11        0.2760           91.8156       0.5584
12        0.4669          148.4332       0.5359
13        0.4311          125.3532       0.5641
14        0.1671          104.6547       0.5498
15        0.3604          101.1515       0.2217

$Best.nc
               KL      CH Hartigan     CCC    Scott  Marriot   TrCovW   TraceW Friedman
Rubin Cindex     DB Silhouette
Number_clusters  2.0000   3.0000   3.0000  2.0000   3.0000     3.00     3.00   3.0000
12.0000  3.0000 8.0000 2.0000     2.0000
Value_Index     73.0541 467.3302 138.8636 -1.6821 430.5103 39619.21 91884.74
131.1384   1.9647 -0.2131 0.1363 0.7704     0.5675
             Duda PseudoT2  Beale Ratkowsky     Ball PtBiserial   Frey McClain   Dunn
Hubert SDindex Dindex    SDbw
Number_clusters 2.0000   2.0000 2.0000    3.0000   3.0000     2.0000 2.0000  2.0000
2.0000      0  2.0000      0 15.0000
Value_Index     0.6122 328.0795 0.6321    0.4534 186.8476     0.6754 3.9697  0.0992
0.0402      0  3.3122      0  0.2749

$Best.partition
  OSR_1   OSR_2   OSR_3   OSR_4   OSR_5   OSR_6   OSR_7   OSR_8   OSR_9  OSR_10
OSR_11   OSR_12   OSR_13   OSR_14
      1       1       1       1       1       1       1       1       1       1       1       1       1       1
```

OSR_15 OSR_16 OSR_17 OSR_18 OSR_19 OSR_20 OSR_21 OSR_22 OSR_23
OSR_24 OSR_25 OSR_26 OSR_27 OSR_28
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_29 OSR_30 OSR_31 OSR_32 OSR_33 OSR_34 OSR_35 OSR_36 OSR_37
OSR_38 OSR_39 OSR_40 OSR_41 OSR_42
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_43 OSR_44 OSR_45 OSR_46 OSR_47 OSR_48 OSR_49 OSR_50 OSR_51
OSR_52 OSR_53 OSR_54 OSR_55 OSR_56
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_57 OSR_58 OSR_59 OSR_60 OSR_61 OSR_62 OSR_63 OSR_64 OSR_65
OSR_66 OSR_67 OSR_68 OSR_69 OSR_70
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_71 OSR_72 OSR_73 OSR_74 OSR_75 OSR_76 OSR_77 OSR_78 OSR_79
OSR_80 OSR_81 OSR_82 OSR_83 OSR_84
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_85 OSR_86 OSR_87 OSR_88 OSR_89 OSR_90 OSR_91 OSR_92 OSR_93
OSR_94 OSR_95 OSR_96 OSR_97 OSR_98
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_99 OSR_100 OSR_101 OSR_102 OSR_103 OSR_104 OSR_105 OSR_106
OSR_107 OSR_108 OSR_109 OSR_110 OSR_111 OSR_112
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_113 OSR_114 OSR_115 OSR_116 OSR_117 OSR_118 OSR_119 OSR_120
OSR_121 OSR_122 OSR_123 OSR_124 OSR_125 OSR_126
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_127 OSR_128 OSR_129 OSR_130 OSR_131 OSR_132 OSR_133 OSR_134
OSR_135 OSR_136 OSR_137 OSR_138 OSR_139 OSR_140
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_141 OSR_142 OSR_143 OSR_144 OSR_145 OSR_146 OSR_147 OSR_148
OSR_149 OSR_150 OSR_151 OSR_152 OSR_153 OSR_154
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_155 OSR_156 OSR_157 OSR_158 OSR_159 OSR_160 OSR_161 OSR_162
OSR_163 OSR_164 OSR_165 OSR_166 OSR_167 OSR_168
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_169 OSR_170 OSR_171 OSR_172 OSR_173 OSR_174 OSR_175 OSR_176
OSR_177 OSR_178 OSR_179 OSR_180 OSR_181 OSR_182
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_183 OSR_184 OSR_185 OSR_186 OSR_388 OSR_389 OSR_390 OSR_489
OSR_490 OSR_491 OSR_492 OSR_493 OSR_494 OSR_495
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_496 OSR_497 OSR_498 OSR_499 OSR_500 OSR_501 OSR_502 OSR_503
OSR_504 OSR_505 OSR_506 OSR_507 OSR_508 OSR_509
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_510 OSR_511 OSR_520 OSR_521 OSR_522 OSR_523 OSR_524 OSR_525
OSR_538 OSR_539 OSR_540 OSR_541 OSR_542 OSR_543
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_544 OSR_545 OSR_546 OSR_547 OSR_548 OSR_549 OSR_550 OSR_551
OSR_552 OSR_634 OSR_635 OSR_636 OSR_639 OSR_647
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_648 OSR_649 OSR_650 OSR_651 OSR_652 OSR_653 OSR_654 OSR_655
OSR_656 OSR_657 OSR_658 OSR_659 OSR_749 OSR_831

1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_832 OSR_833 OSR_834 OSR_835 OSR_836 OSR_837 OSR_838 OSR_839
OSR_841 OSR_842 OSR_843 OSR_844 OSR_846 OSR_847
1 2 1 1 1 1 1 1 1 1 1 1 1 1
OSR_849 OSR_850 OSR_851 OSR_852 OSR_853 OSR_854 OSR_855 OSR_856
OSR_857 OSR_858 OSR_859 OSR_860 OSR_861 OSR_862
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_863 OSR_864 OSR_865 OSR_866 OSR_867 OSR_868 OSR_869 OSR_870
OSR_871 OSR_872 OSR_873 OSR_874 OSR_875 OSR_876
1 1 1 1 1 1 1 1 1 1 1 1 1 2
OSR_877 OSR_878 OSR_880 OSR_881 OSR_882 OSR_884 OSR_886 OSR_887
OSR_888 OSR_889 OSR_890 OSR_891 OSR_892 OSR_893
1 1 1 1 2 1 1 1 1 1 1 1 2 1
OSR_894 OSR_895 OSR_896 OSR_898 OSR_899 OSR_900 OSR_901 OSR_902
OSR_903 OSR_904 OSR_924 OSR_925 OSR_947 OSR_960
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_962 OSR_969 OSR_970 OSR_971 OSR_972 OSR_973 OSR_974 OSR_975
OSR_976 OSR_977 OSR_978 OSR_979 OSR_980 OSR_981
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_982 OSR_983 OSR_984 OSR_985 OSR_986 OSR_987 OSR_988 OSR_989
OSR_990 OSR_991 OSR_992 OSR_993 OSR_994 OSR_995
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_996 OSR_997 OSR_998 OSR_999 OSR_1000 OSR_1001 OSR_1002 OSR_1003
OSR_1004 OSR_1005 OSR_1006 OSR_1007 OSR_1008 OSR_1009
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1010 OSR_1011 OSR_1012 OSR_1013 OSR_1014 OSR_1015 OSR_1016 OSR_1098
OSR_1099 OSR_1100 OSR_1101 OSR_1102 OSR_1103 OSR_1105
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1106 OSR_1107 OSR_1108 OSR_1109 OSR_1110 OSR_1111 OSR_1112 OSR_1113
OSR_1114 OSR_1115 OSR_1116 OSR_1118 OSR_1119 OSR_1123
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1124 OSR_1126 OSR_1127 OSR_1128 OSR_1129 OSR_1130 OSR_1131 OSR_1133
OSR_1134 OSR_1136 OSR_1137 OSR_1138 OSR_1139 OSR_1350
1 1 1 1 1 1 2 1 1 1 1 1 1 1
OSR_1351 OSR_1352 OSR_1353 OSR_1354 OSR_1355 OSR_1356 OSR_1357 OSR_1358
OSR_1359 OSR_1360 OSR_1361 OSR_1362 OSR_1364 OSR_1365
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1367 OSR_1368 OSR_1369 OSR_1370 OSR_1371 OSR_1372 OSR_1373 OSR_1374
OSR_1375 OSR_1376 OSR_1377 OSR_1378 OSR_1379 OSR_1380
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1381 OSR_1382 OSR_1383 OSR_1384 OSR_1385 OSR_1386 OSR_1387 OSR_1388
OSR_1389 OSR_1390 OSR_1391 OSR_1392 OSR_1393 OSR_1403
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_1404 OSR_1829 OSR_1830 OSR_1831 OSR_1832 OSR_1833 OSR_1834 OSR_1835
OSR_1836 OSR_1837 OSR_1838 OSR_1839 OSR_1840 OSR_1841
1 2 2 1 1 1 2 1 1 2 2 2 1 1
OSR_1842 OSR_1843 OSR_1844 OSR_1845 OSR_1846 OSR_1847 OSR_1848 OSR_1849
OSR_1850 OSR_1851 OSR_1852 OSR_1853 OSR_1854 OSR_1855
1 1 1 2 1 1 2 2 2 2 2 2 2 1

OSR_1856 OSR_1857 OSR_1858 OSR_1859 OSR_1860 OSR_1861 OSR_1862 OSR_1863 OSR_1864 OSR_1865 OSR_1866 OSR_1867 OSR_1868 OSR_1869
1 2 2 2 1 2 2 2 2 2 2 2 2 2
OSR_1870 OSR_1871 OSR_1872 OSR_1873 OSR_1874 OSR_1875 OSR_1876 OSR_1877 OSR_1878 OSR_1879 OSR_1880 OSR_1881 OSR_1882 OSR_1883
2 2 2 2 2 2 1 2 2 2 2 2 2 2
OSR_1884 OSR_1885 OSR_1886 OSR_1887 OSR_1888 OSR_1889 OSR_1890 OSR_1891 OSR_1892 OSR_1893 OSR_1894 OSR_1895 OSR_1896 OSR_1920
2 2 2 2 2 2 2 2 2 2 2 2 2 2
OSR_1921 OSR_1922 OSR_1923 OSR_1924 OSR_1925 OSR_1926 OSR_1927 OSR_1928 OSR_1929 OSR_1930 OSR_1931 OSR_1932 OSR_1933 OSR_1934
2 2 1 2 2 1 1 1 1 2 1 1 1 1
OSR_1935 OSR_1936 OSR_1937 OSR_1938 OSR_1939 OSR_1998 OSR_1999 OSR_2000 OSR_2001 OSR_2002 OSR_2003 OSR_2004 OSR_2005 OSR_2006
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_2007 OSR_2008 OSR_2009 OSR_2010 OSR_2011 OSR_2012 OSR_2013 OSR_2014 OSR_2015 OSR_2016 OSR_2017 OSR_2018 OSR_2019 OSR_2020
1 2 1 1 1 1 1 1 1 1 1 1 1 1
OSR_2021 OSR_2022 OSR_2023 OSR_2024 OSR_2025 OSR_2026 OSR_2027 OSR_2028 OSR_2029 OSR_2030 OSR_2031 OSR_2034 OSR_2035 OSR_2036
1 1 1 1 1 1 1 1 1 1 1 1 1 1
OSR_2037 OSR_2038 OSR_2039 OSR_2040 OSR_2041 OSR_2042 OSR_2043 OSR_2044 OSR_2045 OSR_2046
1 1 1 1 1 1 1 1 1 1

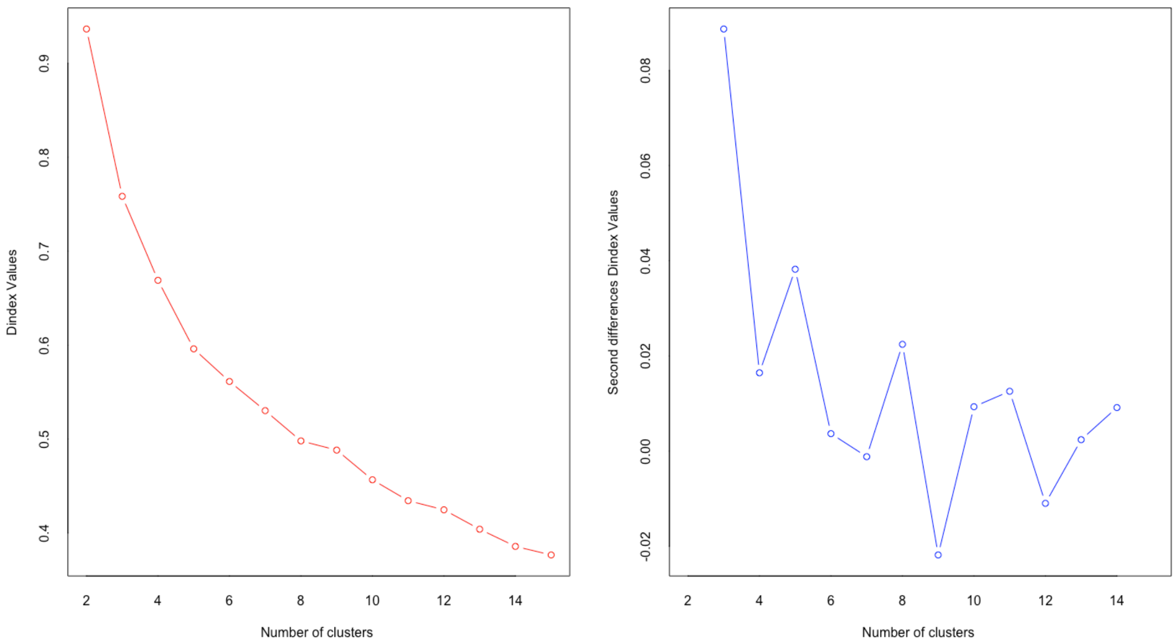


Figure F-9: Hierarchical clustering of enamel δ13C and δ18O data D-index outputs for optimal clusters.

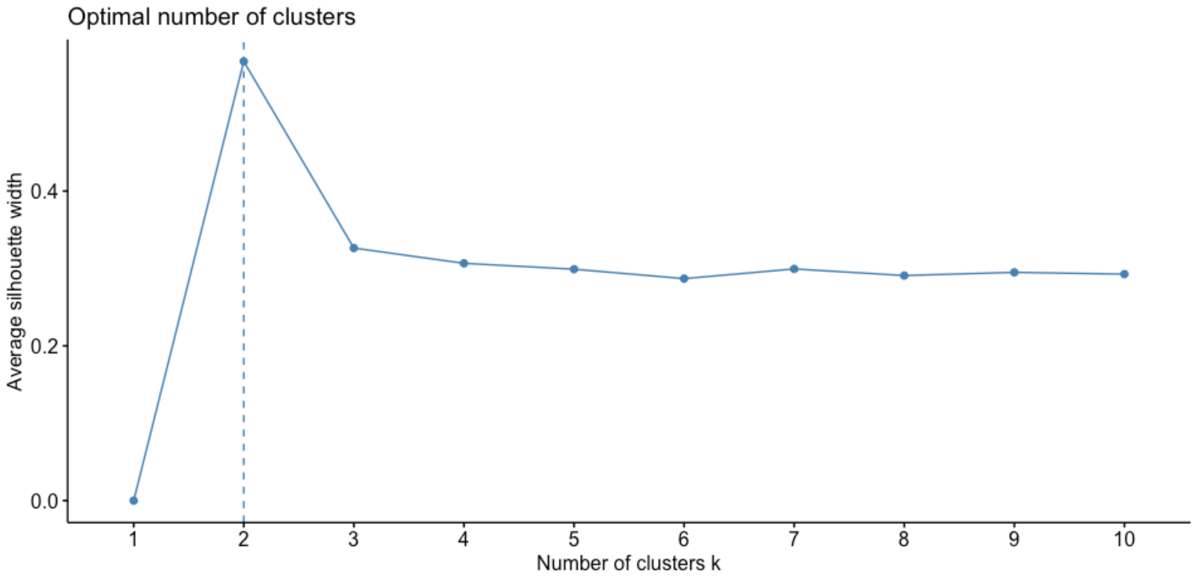


Figure F-10: Silhouette method for optimal number of hierarchical clusters for enamel δ[13]C and δ[18]O.

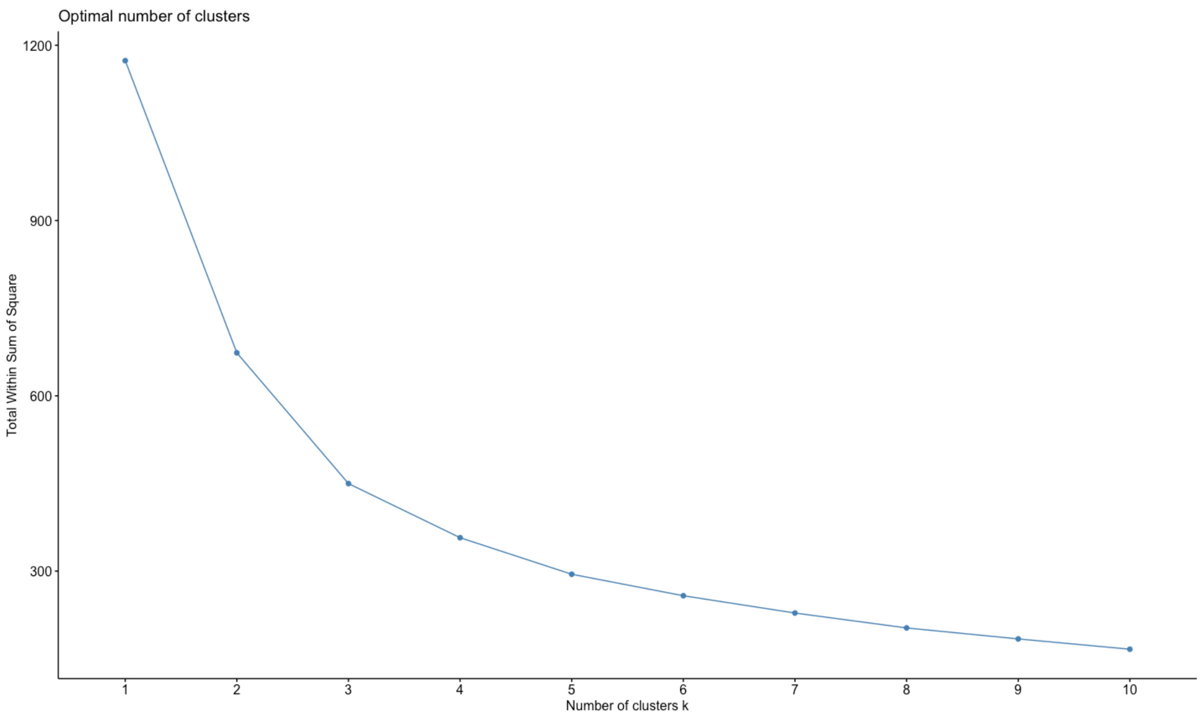


Figure F-11: Elbow method for optimal number of hierarchical clusters for enamel δ[13]C and δ[18]O.

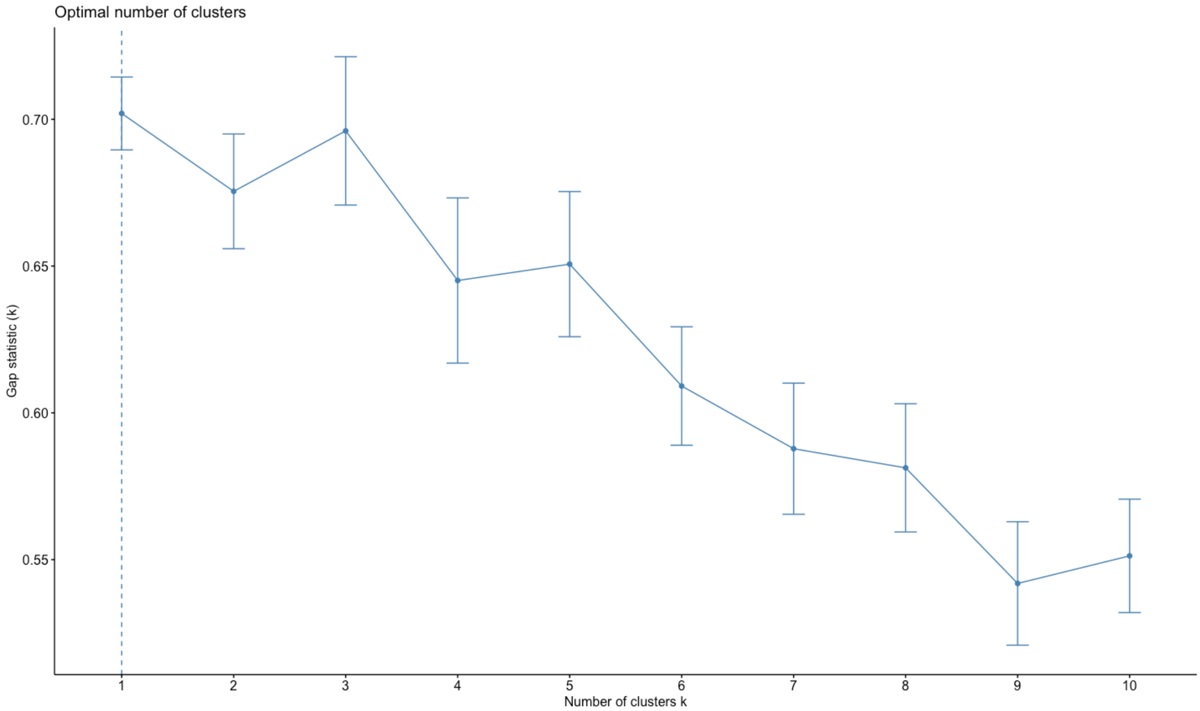


Figure F-12: Gap statistic method for optimal number of hierarchical clusters for enamel δ13C and δ18O.

F.iv Bone

NbClust(data = EMEUboneclean, diss = NULL, distance = "euclidean", min.nc = 2, max.nc = 15, method = "ward.D2")
*** : The Hubert index is a graphical method of determining the number of clusters.
In the plot of Hubert index, we seek a significant knee that corresponds to a
significant increase of the value of the measure i.e the significant peak in
Hubert
index second differences plot.

*** : The D index is a graphical method of determining the number of clusters.
In the plot of D index, we seek a significant knee (the significant peak in
Dindex
second differences plot) that corresponds to a significant increase of the value
of
the measure.

****
* Among all indices:
* 3 proposed 2 as the best number of clusters
* 8 proposed 3 as the best number of clusters
* 2 proposed 4 as the best number of clusters
* 1 proposed 5 as the best number of clusters
* 6 proposed 6 as the best number of clusters
* 1 proposed 7 as the best number of clusters
* 1 proposed 12 as the best number of clusters
* 1 proposed 15 as the best number of clusters

***** Conclusion *****

* According to the majority rule, the best number of clusters is 3

```
*******************************************************************
$All.index
     KL      CH  Hartigan     CCC     Scott  Marriot     TrCovW   TraceW Friedman  Rubin
Cindex    DB Silhouette   Duda
2  2.9470 1923.879 1552.1379 -22.9149  3595.199 28062699 10559187.3 5648.984
1.3085 1.4650 0.1413 1.4502     0.3921 0.5151
3  5.2031 2098.406 1291.8626 -42.5995  5804.395 37025991  3765891.2 4107.801
2.1228 2.0147 0.1388 1.0617     0.4075 0.6043
4  1.1856 2265.962  966.0241 -38.5583  8121.882 37602469  1738443.2 3130.121
3.4543 2.6440 0.1565 1.0465     0.3121 0.5344
5  1.5564 2337.445  868.9175 -36.8777  9827.143 38914172  1151233.5 2537.343
4.6931 3.2617 0.1441 1.0428     0.3162 0.5629
6  0.1082 2436.193  337.8742 -34.5102 11286.202 39389006   999386.8 2096.652
5.9249 3.9472 0.1183 1.1218     0.3068 0.6733
7  1.4673 2251.894  367.1101 -39.2452 12000.497 45114845   707889.5 1938.203
6.6749 4.2699 0.1106 1.1897     0.2896 0.5654
8  1.3385 2153.608  357.8757 -41.9811 12646.659 50408444   677554.7 1780.053
7.3405 4.6493 0.1221 1.1786     0.2866 0.6735
9  1.1280 2091.884  324.2138 -43.8069 13311.730 54328058   677271.5 1638.139
8.1065 5.0521 0.1205 1.1299     0.2902 0.5711
10 2.0277 2040.953  348.1011 -45.3730 13966.314 57260534   512580.7 1518.902
8.9695 5.4487 0.1156 1.1308     0.2811 0.5685
11 2.1568 2026.036  345.6806 -45.9072 14668.331 58476296   378339.8 1400.805
9.9641 5.9080 0.1138 1.0910     0.2821 0.4325
12 2.0891 2027.022  329.8978 -45.9650 15291.359 59866562   370837.8 1292.565
10.8585 6.4028 0.1462 1.0017     0.2826 0.6694
13 1.2932 2033.633  328.1841 -45.8458 15957.638 59813276   287846.6 1196.890
11.9718 6.9146 0.1411 1.0205     0.2557 0.6409
14 0.2107 2051.260  244.2454 -45.3911 16548.071 60147063   285571.4 1108.703
12.9476 7.4646 0.1323 1.0586     0.2523 0.5438
15 1.7699 2034.476  246.7738 -45.9523 17020.621 61596685   281030.2 1046.725
13.8212 7.9066 0.1260 1.0494     0.2570 0.5299
   Pseudot2  Beale Ratkowsky     Ball Ptbiserial    Frey McClain   Dunn Hubert SDindex
Dindex   SDbw
2  1146.7191 0.9407    0.3673 2824.4922     0.4729 -0.4888  0.3803 0.0067  2e-04
6.3540 0.9403 1.4088
3  1910.0016 0.6546    0.4087 1369.2671     0.5423  1.7266  0.3885 0.0072  2e-04
4.5541 0.8232 0.8481
4   816.4711 0.8704    0.3940  782.5302     0.4589  0.0132  0.9319 0.0040  2e-04
4.4837 0.7153 0.9543
5  1518.3939 0.7763    0.3723  507.4687     0.4816  0.6693  0.9502 0.0040  3e-04
4.0522 0.6508 0.7618
6   465.7589 0.4847    0.3528  349.4420     0.4437  0.4731  1.3848 0.0040  3e-04
4.2693 0.5742 0.6447
7   214.4304 0.7658    0.3308  276.8862     0.4345  0.0040  1.5027 0.0040  3e-04
4.9696 0.5426 0.5867
```

```
8   142.5110 0.4831    0.3132  222.5067     0.4371 -0.0846  1.4936 0.0044  3e-04
4.8725 0.5256 0.5206
9   491.1249 0.7498    0.2985  182.0154     0.4397  0.4829  1.4809 0.0044  3e-04
4.6677 0.5135 0.4678
10  202.6979 0.7563    0.2857  151.8902     0.4331  0.0175  1.5512 0.0044  3e-04
4.6145 0.4920 0.4626
11  356.9464 1.3075    0.2748  127.3459     0.4349 -0.1083  1.5427 0.0044  3e-04
4.3367 0.4798 0.4260
12  641.5641 0.4935    0.2652  107.7137     0.4367  2.3670  1.5319 0.0058  3e-04
5.5693 0.4732 0.4464
13  359.1052 0.5594    0.2565   92.0684     0.3687  0.2772  2.2394 0.0058  4e-04
7.0510 0.4486 0.4399
14  575.4163 0.8376    0.2487   79.1931     0.3624  0.3663  2.3322 0.0058  4e-04
7.1806 0.4299 0.4010
15  187.1673 0.8829    0.2413   69.7817     0.3544  0.0838  2.4430 0.0058  4e-04
7.1968 0.4162 0.3780

$All.CriticalValues
  CritValue_Duda CritValue_PseudoT2 Fvalue_Beale
2         0.6110          775.3291       0.3905
3         0.6360         1669.3758       0.5197
4         0.6012          621.6597       0.4189
5         0.6259         1168.4713       0.4602
6         0.6021          634.3506       0.6160
7         0.5345          243.0072       0.4654
8         0.5383          252.2106       0.6171
9         0.5853          463.2995       0.4727
10        0.5312          235.6094       0.4699
11        0.5326          238.6958       0.2713
12        0.6133          819.1438       0.6105
13        0.5844          455.9063       0.5717
14        0.5876          481.4464       0.4330
15        0.5126          200.6259       0.4144

$Best.nc
               KL      CH Hartigan      CCC    Scott Marriot  TrCovW   TraceW Friedman
Rubin Cindex      DB Silhouette
Number_clusters 3.0000    6.000   6.0000   2.0000    4.000       6      3   3.0000   4.0000
6.0000 7.0000 12.0000     3.0000
Value_Index     5.2031 2436.193 531.0433 -22.9149 2317.486 5251004 6793296
563.5026   1.3315 -0.3629 0.1106  1.0017     0.4075
              Duda PseudoT2  Beale Ratkowsky     Ball PtBiserial Frey McClain   Dunn
Hubert SDindex Dindex   SDbw
Number_clusters 6.0000   6.0000 2.0000    3.0000    3.000     3.0000    1  2.0000 3.0000
0  5.0000      0 15.000
Value_Index     0.6733 465.7589 0.9407    0.4087 1455.225     0.5423   NA  0.3803
0.0072      0  4.0522      0  0.378

$Best.partition TOO MANY TO PRINT
```

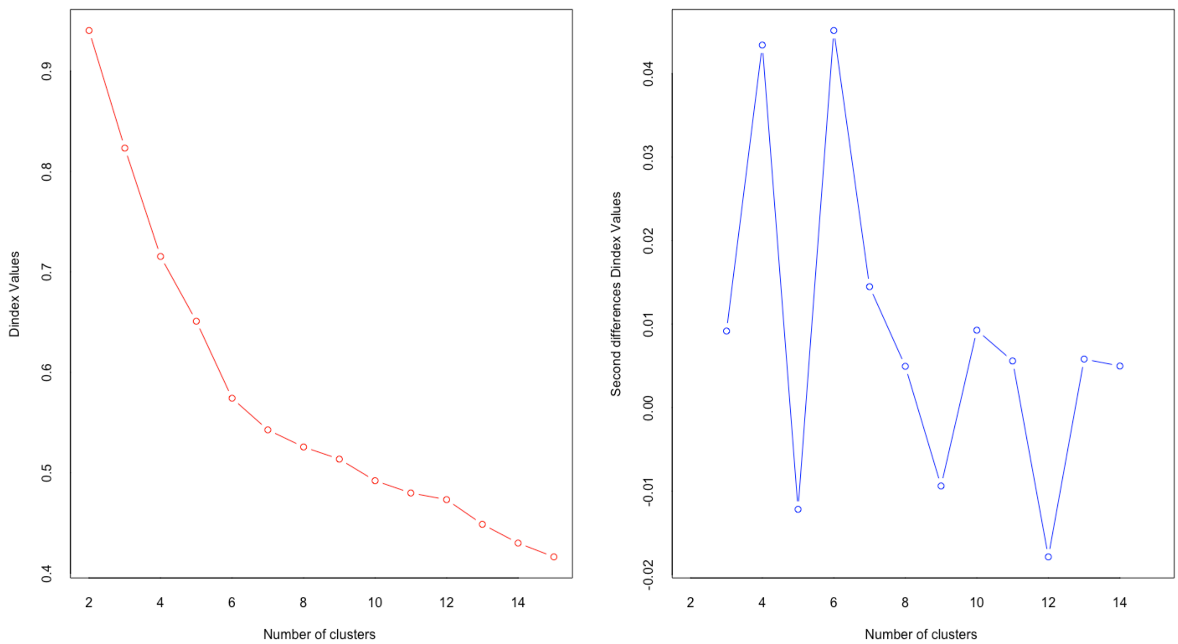


Figure F-13: Hierarchical clustering of bone isotope data D-index outputs for optimal clusters.

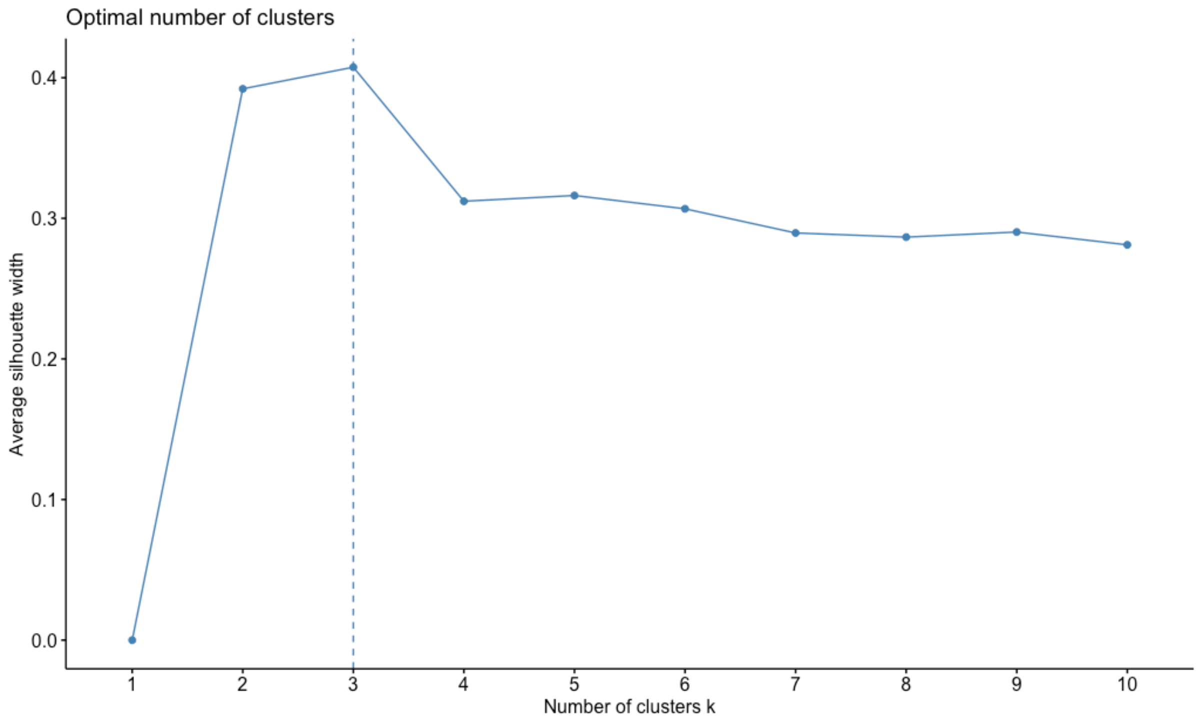


Figure F-14: Silhouette method for optimal number of hierarchical clusters for bone $\delta^{13}C$ and $\delta^{15}N$.

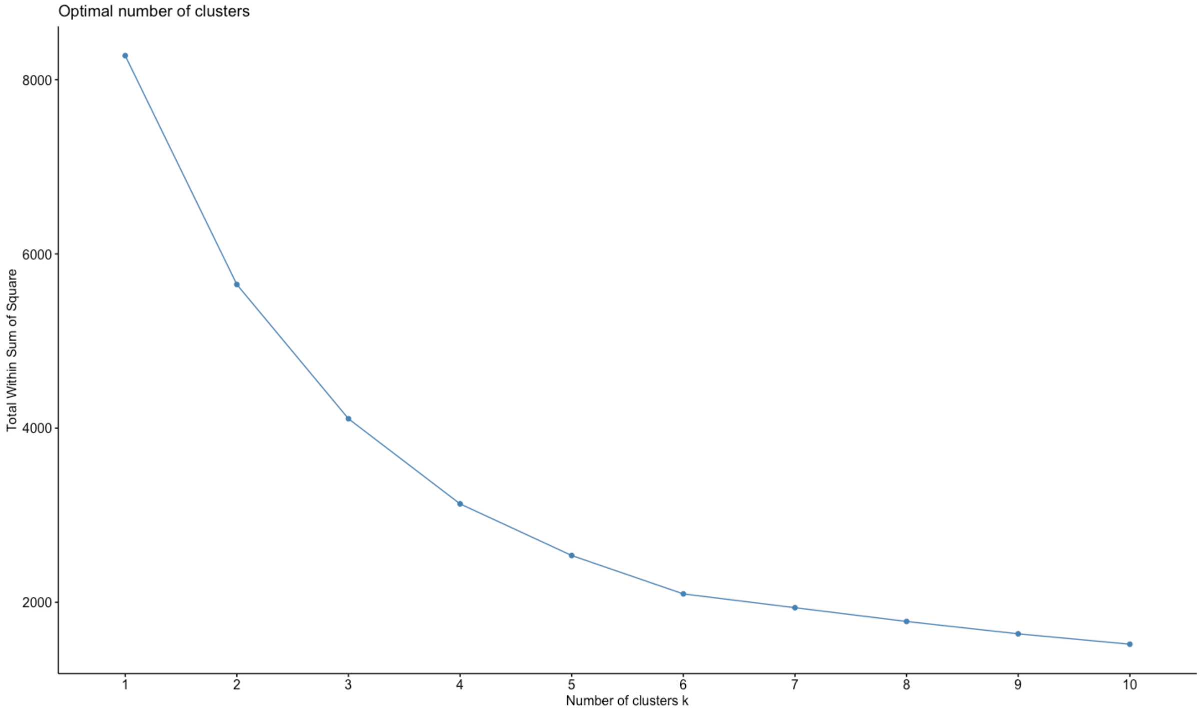


Figure F-15: Elbow method for optimal number of hierarchical clusters for bone $\delta^{13}C$ and $\delta^{15}N$.

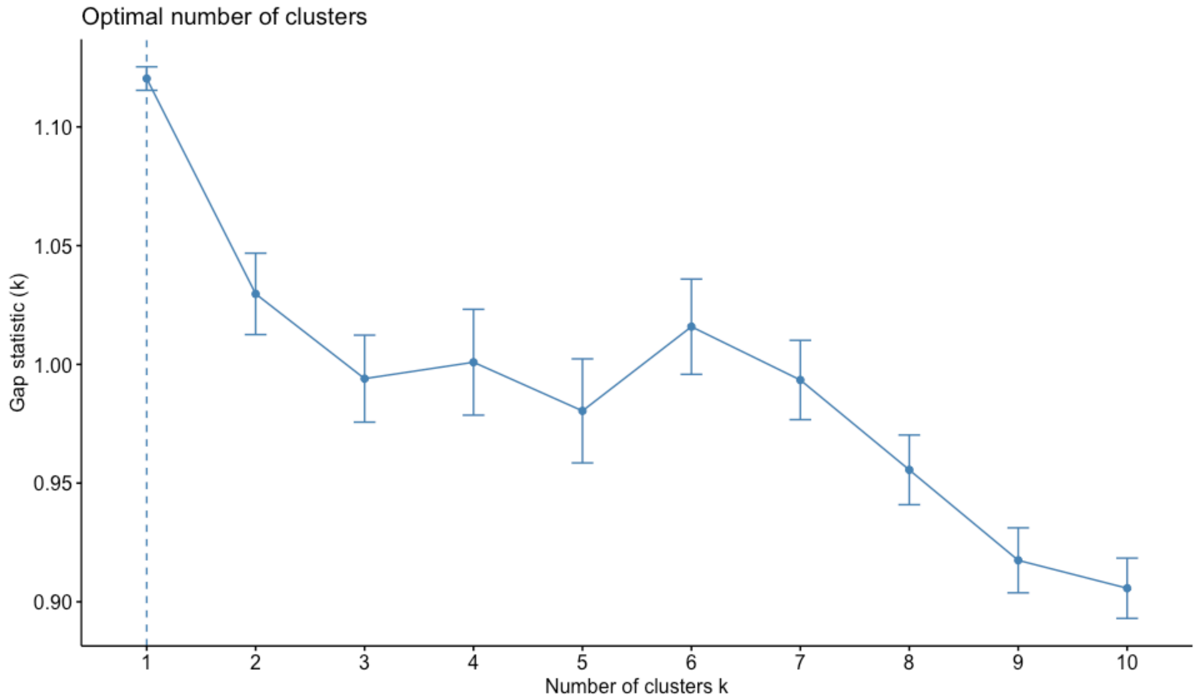


Figure F-16: Gap statistic method for optimal number of hierarchical clusters for bone $\delta^{13}C$ and $\delta^{15}N$.

F.v Dentine

NbClust(data = EMEUdentineclean, diss = NULL, distance = "euclidean", min.nc = 2, max.nc = 15, method = "ward.D2")

*** : The Hubert index is a graphical method of determining the number of clusters.
In the plot of Hubert index, we seek a significant knee that corresponds to a significant increase of the value of the measure i.e the significant peak in Hubert
index second differences plot.

*** : The D index is a graphical method of determining the number of clusters.
In the plot of D index, we seek a significant knee (the significant peak in Dindex
second differences plot) that corresponds to a significant increase of the value of
the measure.

****
* Among all indices:
* 1 proposed 2 as the best number of clusters
* 11 proposed 3 as the best number of clusters
* 2 proposed 4 as the best number of clusters
* 5 proposed 5 as the best number of clusters
* 2 proposed 11 as the best number of clusters
* 1 proposed 13 as the best number of clusters
* 1 proposed 15 as the best number of clusters

***** Conclusion *****

* According to the majority rule, the best number of clusters is 3

****
$All.index
KL CH Hartigan CCC Scott Marriot TrCovW TraceW Friedman Rubin
Cindex DB Silhouette Duda
2 1.1605 689.8837 638.3127 -3.0678 1164.951 943438.6 512552.084 1067.3651
1.9708 1.7426 0.1490 1.1517 0.4481 0.4261
3 2.6473 900.1366 253.6577 -2.3540 1970.244 893803.0 92376.167 632.6639
3.9210 2.9399 0.1860 0.7636 0.4883 0.5277
4 0.7343 847.7568 307.3965 -4.1147 2462.697 936265.0 91811.213 496.8547
5.7963 3.7435 0.2032 0.8730 0.4005 0.6008
5 1.0312 922.5099 119.0435 -1.4182 3000.736 820792.8 36394.359 373.1251
8.5692 4.9849 0.1680 0.9714 0.3386 0.6702
6 1.0541 855.7673 96.4745 -3.7506 3272.885 882355.4 22899.105 330.6215
10.5059 5.6258 0.1540 1.1333 0.2984 0.6277
7 1.3558 802.7278 91.9402 -5.7153 3483.187 958153.5 14718.625 299.3955
12.1124 6.2125 0.1442 1.1617 0.2933 0.4261
8 1.9342 768.8166 95.4013 -7.0374 3623.368 1076532.1 14011.121 272.3009
12.9927 6.8307 0.1390 1.0359 0.2830 0.6240
9 0.8749 753.3544 80.4051 -7.6688 3840.429 1079138.0 8810.811 246.7924
15.0569 7.5367 0.1321 1.1063 0.2787 0.4945
10 2.5513 736.1811 83.6286 -8.3866 3959.482 1172345.9 7775.685 226.9967
15.8773 8.1940 0.1264 1.0674 0.2896 0.6703
11 6.6935 730.2941 82.3841 -8.6536 4093.848 1227897.2 7708.636 208.1007
17.0057 8.9380 0.1171 1.0821 0.2998 0.5143
12 0.1012 730.0500 89.0134 -8.6907 4231.375 1260623.2 6410.307 190.9973
18.2310 9.7384 0.1633 1.0967 0.2933 0.4115
13 0.5441 740.6428 93.8351 -8.2839 4379.846 1261393.5 6026.755 174.1311
19.6721 10.6816 0.2065 1.0337 0.2956 0.5413

```
14 1.2512 759.9423  84.2959 -7.5343 4561.080 1204142.0   5887.249  157.9826
21.9124 11.7734 0.1913 1.0063     0.2988 0.5232
15 1.6569 775.7033  72.4795 -6.9416 4712.309 1175055.7   5004.047  144.6826
23.7635 12.8557 0.1802 0.9768     0.3089 0.3920
   Pseudot2  Beale Ratkowsky     Ball Ptbiserial    Frey McClain   Dunn Hubert SDindex
Dindex   SDbw
2  507.7796 1.3433    0.4536 533.6826     0.4960 -0.5753  0.4751 0.0062 0.0007
3.9937 0.8394 1.2743
3  307.0376 0.8926    0.4689 210.8880     0.6042  1.1814  0.4414 0.0090 0.0011
2.9269 0.7184 0.6612
4  365.4913 0.6633    0.4280 124.2137     0.5918  1.4329  0.5445 0.0106 0.0012
2.9958 0.6352 0.5551
5  180.1015 0.4907    0.3997  74.6250     0.5044  1.6433  1.0051 0.0105 0.0013  3.3165
0.5475 0.5778
6  132.8464 0.5904    0.3700  55.1036     0.4357  0.6402  1.4856 0.0105 0.0014  4.5300
0.5036 0.4619
7  290.8936 1.3405    0.3461  42.7708     0.4183  1.5417  1.6717 0.0105 0.0014  4.5532
0.4793 0.5807
8   70.5056 0.5975    0.3266  34.0376     0.3855  0.2080  2.0231 0.0105 0.0014  4.5331
0.4476 0.6078
9  151.2832 1.0153    0.3104  27.4214     0.3838  0.4343  2.0624 0.0105 0.0014  4.3006
0.4303 0.4894
10  89.5206 0.4892    0.2963  22.6997     0.3753  0.3896  2.1756 0.0105 0.0014  4.8752
0.4102 0.4409
11  30.2145 0.9156    0.2841  18.9182     0.3621  0.0127  2.3532 0.0105 0.0015  4.7917
0.3952 0.4127
12  70.0885 1.4018    0.2734  15.9164     0.3629  0.0078  2.3400 0.0148 0.0015  4.8309
0.3876 0.3185
13 130.5143 0.8420    0.2640  13.3947     0.3641  0.3873  2.3210 0.0190 0.0015
4.5056 0.3772 0.2832
14 122.1056 0.9045    0.2557  11.2845     0.3503  0.1081  2.4950 0.0190 0.0015
4.6258 0.3560 0.2872
15 105.4624 1.5284    0.2480   9.6455     0.3501  0.2101  2.4658 0.0190 0.0015  4.7841
0.3452 0.2635

$All.CriticalValues
   CritValue_Duda CritValue_PseudoT2 Fvalue_Beale
2          0.5549           302.3658       0.2616
3          0.5488           281.9660       0.4101
4          0.5767           403.7767       0.5153
5          0.5530           295.7861       0.6124
6          0.5175           208.8197       0.5545
7          0.5146           203.7829       0.2628
8          0.4555           139.8775       0.5510
9          0.4802           160.2064       0.3635
10         0.4998           182.1721       0.6135
11         0.2585            91.8049       0.4055
12         0.3361            96.7755       0.2511
13         0.4841           164.1092       0.4318
14         0.4701           151.0575       0.4060
```

15 0.3867 107.8309 0.2206

$Best.nc
KL CH Hartigan CCC Scott Marriot TrCovW TraceW Friedman
Rubin Cindex DB
Number_clusters 11.0000 5.0000 3.000 5.0000 3.0000 5.0 3.0 3.0000
5.0000 5.0000 11.0000 3.0000
Value_Index 6.6935 922.5099 384.655 -1.4182 805.2928 177034.9 420175.9
298.8919 2.7728 -0.6005 0.1171 0.7636
Silhouette Duda PseudoT2 Beale Ratkowsky Ball PtBiserial Frey McClain
Dunn Hubert SDindex Dindex
Number_clusters 3.0000 4.0000 4.0000 2.0000 3.0000 3.0000 3.0000 1
3.0000 13.000 0 3.0000 0
Value_Index 0.4883 0.6008 365.4913 1.3433 0.4689 322.7946 0.6042 NA
0.4414 0.019 0 2.9269 0
SDbw
Number_clusters 15.0000
Value_Index 0.2635

$Best.partition
CND_01 CND_02 CND_03 CND_04 CND_05 CND_06 CND_07 CND_08 CND_09
CND_10 CND_11 CND_12 CND_13 CND_14 CND_15 CND_16
1 1 1 1 1 1 1 2 1 1 2 2 2 2 2 2
CND_17 CND_18 CND_19 CND_20 CND_21 CND_22 CND_23 CND_24 CND_25
CND_26 CND_27 CND_28 CND_29 CND_30 CND_31 CND_32
2 2 2 2 2 2 2 1 2 2 2 2 2 2 2 2
CND_33 CND_34 CND_35 CND_36 CND_37 CND_38 CND_39 CND_40 CND_41
CND_42 CND_43 CND_44 CND_45 CND_46 CND_47 CND_48
2 2 2 2 2 2 2 2 1 2 2 2 2 2 1 1
CND_49 CND_50 CND_51 CND_52 CND_53 CND_54 CND_55 CND_56 CND_57
CND_58 CND_59 CND_60 CND_61 CND_62 CND_63 CND_64
1 2 2 2 1 2 2 2 2 2 2 2 2 2 2 2
CND_65 CND_66 CND_67 CND_68 CND_69 CND_70 CND_71 CND_72 CND_73
CND_74 CND_75 CND_76 CND_77 CND_78 CND_79 CND_80
2 2 2 1 1 1 2 2 2 1 2 2 1 2 1 1
CND_81 CND_82 CND_83 CND_84 CND_85 CND_86 CND_87 CND_88 CND_89
CND_90 CND_91 CND_92 CND_93 CND_94 CND_95 CND_96
1 2 2 1 1 1 1 1 1 1 1 1 1 2 2 2
CND_97 CND_98 CND_99 CND_100 CND_101 CND_102 CND_103 CND_104 CND_105
CND_106 CND_107 CND_108 CND_109 CND_110 CND_111 CND_112
2 2 2 1 2 2 1 1 1 2 1 1 1 1 1 1
CND_113 CND_114 CND_115 CND_116 CND_117 CND_118 CND_119 CND_120
CND_121 CND_122 CND_123 CND_124 CND_125 CND_126 CND_127 CND_128
1 1 1 1 1 1 1 1 1 2 2 2 2 1 1 2
CND_129 CND_130 CND_131 CND_132 CND_133 CND_134 CND_135 CND_136
CND_137 CND_138 CND_139 CND_140 CND_141 CND_142 CND_143 CND_144
2 1 1 1 2 2 2 1 1 1 2 2 2 1 2 1
CND_145 CND_146 CND_147 CND_148 CND_149 CND_150 CND_151 CND_152
CND_153 CND_154 CND_155 CND_156 CND_157 CND_158 CND_159 CND_160
1 1 1 1 2 2 2 1 1 1 2 2 2 1 1 1

CND_161 CND_162 CND_163 CND_164 CND_165 CND_166 CND_167 CND_168
CND_169 CND_170 CND_171 CND_172 CND_173 CND_174 CND_175 CND_176
1 1 1 2 1 1 1 1 1 1 1 1 1 1 1 2
CND_177 CND_178 CND_179 CND_180 CND_181 CND_182 CND_183 CND_184
CND_185 CND_186 CND_187 CND_188 CND_189 CND_190 CND_191 CND_192
2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_193 CND_194 CND_195 CND_196 CND_197 CND_198 CND_199 CND_200
CND_201 CND_202 CND_203 CND_204 CND_205 CND_206 CND_207 CND_208
1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 1
CND_209 CND_210 CND_211 CND_212 CND_213 CND_214 CND_215 CND_216
CND_217 CND_218 CND_219 CND_220 CND_221 CND_222 CND_223 CND_224
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_225 CND_226 CND_227 CND_228 CND_229 CND_230 CND_231 CND_232
CND_233 CND_234 CND_235 CND_236 CND_237 CND_238 CND_239 CND_240
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_241 CND_242 CND_243 CND_244 CND_245 CND_246 CND_247 CND_248
CND_249 CND_250 CND_251 CND_252 CND_253 CND_254 CND_255 CND_256
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_257 CND_258 CND_259 CND_260 CND_261 CND_262 CND_263 CND_264
CND_265 CND_266 CND_267 CND_268 CND_269 CND_270 CND_271 CND_272
1 1 1 1 1 1 1 1 1 1 1 1 1 2 1 1
CND_273 CND_274 CND_275 CND_276 CND_277 CND_278 CND_279 CND_280
CND_281 CND_282 CND_283 CND_284 CND_285 CND_286 CND_287 CND_288
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_289 CND_290 CND_291 CND_292 CND_293 CND_294 CND_295 CND_296
CND_297 CND_298 CND_299 CND_300 CND_301 CND_302 CND_303 CND_304
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_305 CND_306 CND_307 CND_308 CND_309 CND_310 CND_311 CND_312
CND_313 CND_314 CND_315 CND_316 CND_317 CND_318 CND_319 CND_320
1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 1
CND_321 CND_322 CND_323 CND_324 CND_325 CND_326 CND_327 CND_328
CND_329 CND_330 CND_331 CND_332 CND_333 CND_334 CND_335 CND_336
1 1 2 1 1 2 1 2 1 1 2 1 1 1 2 2
CND_337 CND_338 CND_339 CND_340 CND_341 CND_342 CND_343 CND_344
CND_345 CND_346 CND_347 CND_348 CND_349 CND_350 CND_351 CND_352
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_353 CND_354 CND_355 CND_356 CND_357 CND_358 CND_359 CND_360
CND_361 CND_362 CND_363 CND_364 CND_365 CND_366 CND_367 CND_368
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_369 CND_370 CND_371 CND_372 CND_373 CND_374 CND_375 CND_376
CND_377 CND_378 CND_379 CND_380 CND_381 CND_382 CND_383 CND_384
1 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_385 CND_386 CND_387 CND_388 CND_389 CND_390 CND_391 CND_392
CND_393 CND_394 CND_395 CND_396 CND_397 CND_398 CND_399 CND_400
2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
CND_401 CND_402 CND_403 CND_404 CND_405 CND_406 CND_407 CND_408
CND_409 CND_410 CND_411 CND_412 CND_413 CND_414 CND_415 CND_416
1 1 1 1 1 1 1 1 1 1 1 2 1 1 1 1
CND_417 CND_418 CND_419 CND_420 CND_421 CND_422 CND_423 CND_424
CND_425 CND_426 CND_427 CND_428 CND_429 CND_430 CND_431 CND_432

```
   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1   1 
CND_433 CND_434 CND_435 CND_436 CND_437 CND_438 CND_439 CND_440 
CND_441 CND_442 CND_443 CND_444 CND_445 CND_446 CND_447 CND_448 
   1   2   1   1   1   1   1   1   1   1   1   1   1   1   1   1 
CND_449 CND_450 CND_451 CND_452 CND_453 CND_454 CND_455 CND_456 
CND_457 CND_458 CND_459 CND_460 CND_461 CND_462 CND_463 CND_464 
   1   1   1   1   1   1   1   1   1   2   1   1   1   1   3   1 
CND_465 CND_466 CND_467 CND_468 CND_469 CND_470 CND_471 CND_472 
CND_473 CND_474 CND_475 CND_476 CND_477 CND_478 CND_479 CND_480 
   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3   3 
CND_481 CND_482 CND_483 CND_484 CND_485 CND_486 CND_487 CND_488 
CND_489 CND_490 CND_491 CND_492 CND_493 CND_494 CND_495 CND_496 
   3   3   3   3   3   3   3   3   3   3   3   3   3   2   2   2 
CND_497 CND_498 CND_499 CND_500 CND_501 CND_502 CND_503 CND_504 
CND_505 CND_506 CND_507 CND_508 CND_509 CND_510 CND_511 CND_512 
   2   1   2   1   1   1   2   2   2   2   2   2   2   2   2   2 
CND_513 CND_514 CND_515 CND_516 CND_517 CND_518 CND_519 CND_520 
CND_521 CND_522 CND_523 CND_524 CND_525 CND_526 CND_527 CND_528 
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2 
CND_529 CND_530 CND_531 CND_532 CND_533 CND_534 CND_535 CND_536 
CND_537 CND_538 CND_539 CND_540 CND_541 CND_542 CND_543 CND_544 
   1   1   1   2   2   2   2   2   2   2   1   2   2   2   2   2 
CND_545 CND_546 CND_547 CND_548 CND_549 CND_550 CND_551 CND_552 
CND_553 CND_554 CND_555 CND_556 CND_557 CND_558 CND_559 CND_560 
   2   2   2   2   2   2   2   2   2   1   1   1   1   1   1   1 
CND_561 CND_562 CND_563 CND_564 CND_565 CND_566 CND_567 CND_568 
CND_569 CND_570 CND_571 CND_572 CND_573 CND_574 CND_575 CND_576 
   2   1   1   1   1   1   1   1   2   1   1   1   2   2   2   2 
CND_577 CND_578 CND_579 CND_580 CND_581 CND_582 CND_583 CND_584 
CND_585 CND_586 CND_587 CND_588 CND_589 CND_590 CND_591 CND_592 
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2 
CND_593 CND_594 CND_595 CND_596 CND_597 CND_598 CND_599 CND_600 
CND_601 CND_602 CND_603 CND_604 CND_605 CND_606 CND_607 CND_608 
   2   2   2   2   2   2   2   1   1   1   1   1   1   1   1   1 
CND_609 CND_610 CND_611 CND_612 CND_613 CND_614 CND_615 CND_616 
CND_617 CND_618 CND_619 CND_620 CND_621 CND_622 CND_623 CND_624 
   1   1   1   1   1   1   1   2   2   2   2   2   2   2   2   2 
CND_625 CND_626 CND_627 CND_628 CND_629 CND_630 CND_631 CND_632 
CND_633 CND_634 CND_635 CND_636 CND_637 CND_638 CND_639 CND_640 
   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2   2 
CND_641 CND_642 CND_643 CND_644 CND_645 CND_646 CND_647 CND_648 
CND_649 CND_650 CND_651 CND_652 CND_653 CND_654 CND_655 CND_656 
   2   2   2   2   2   2   2   1   1   1   2   2   2   2   2   2 
CND_657 CND_658 CND_659 CND_660 CND_661 CND_662 CND_663 CND_664 
CND_665 CND_666 CND_667 CND_668 CND_669 CND_670 CND_671 CND_672 
   2   1   2   2   2   2   2   2   2   2   2   1   1   1   1   1 
CND_673 CND_674 CND_675 CND_676 CND_677 CND_678 CND_679 CND_680 
CND_681 CND_682 CND_683 CND_684 CND_685 CND_686 CND_687 CND_688 
   1   2   2   1   1   1   1   1   1   2   2   2   2   2   2   2 
```

```
CND_689 CND_690 CND_691 CND_692 CND_693 CND_694 CND_695 CND_696 
CND_697 CND_698 CND_699 CND_700 CND_701 CND_702 CND_703 CND_704 
      2       2       2       2       2       2       1       1       1       1       1       1       1       1       2       1 
CND_705 CND_706 CND_707 CND_708 CND_709 CND_710 CND_711 CND_712 
CND_713 CND_714 CND_715 CND_716 CND_717 CND_718 CND_719 CND_720 
      2       1       2       2       1       1       1       1       1       2       1       1       1       1       2       2 
CND_721 CND_722 CND_723 CND_724 CND_725 CND_726 CND_727 CND_728 
CND_729 CND_730 CND_731 CND_732 CND_733 CND_734 CND_735 CND_736 
      2       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2 
CND_737 CND_738 CND_739 CND_740 CND_741 CND_742 CND_743 CND_744 
CND_745 CND_746 CND_747 CND_748 CND_749 CND_750 CND_751 CND_752 
      2       2       2       1       1       1       1       1       1       1       1       1       2       2       1       1 
CND_753 CND_754 CND_755 CND_756 CND_757 CND_758 CND_759 CND_760 
CND_761 CND_762 CND_763 CND_764 CND_765 CND_766 CND_767 CND_768 
      1       1       1       1       2       2       2       2       2       2       2       2       2       2       2       1 
CND_769 CND_770 CND_771 CND_772 CND_773 CND_774 CND_775 CND_776 
CND_777 CND_778 CND_779 CND_780 CND_781 CND_782 CND_783 CND_784 
      1       2       2       2       2       2       2       2       2       2       2       2       2       2       2       2 
CND_785 CND_786 CND_787 CND_788 CND_789 CND_790 CND_791 CND_792 
CND_793 CND_794 CND_795 CND_796 CND_797 CND_798 CND_799 CND_800 
      2       2       2       2       2       2       1       1       1       1       1       1       1       2       2       2 
CND_801 CND_802 CND_803 CND_804 CND_805 CND_806 CND_807 CND_808 
CND_809 CND_810 CND_811 CND_812 CND_813 CND_814 CND_815 CND_816 
      1       1       1       1       1       2       1       2       2       2       2       2       1       1       1       2 
CND_817 CND_818 CND_819 CND_820 CND_821 CND_822 CND_823 CND_824 
CND_825 CND_826 CND_827 CND_828 CND_829 CND_830 CND_831 CND_832 
      1       2       2       2       2       2       2       2       2       2       1       2       1       1       1       1 
CND_833 CND_834 CND_835 CND_836 CND_837 CND_838 CND_839 CND_840 
CND_841 CND_842 CND_843 CND_844 CND_845 CND_846 CND_847 CND_848 
      1       1       2       2       2       1       1       2       2       2       2       1       1       1       1       2 
CND_849 CND_850 CND_851 CND_852 CND_853 CND_854 CND_855 CND_856 
CND_857 CND_858 CND_859 CND_860 CND_861 CND_862 CND_863 CND_864 
      1       1       1       1       1       1       1       1       1       1       1       1       1       1       1       1 
CND_865 CND_866 CND_867 CND_868 CND_869 CND_870 CND_871 CND_872 
CND_873 CND_874 CND_875 CND_876 CND_877 CND_878 CND_879 CND_880 
      1       1       1       1       1       1       1       2       2       2       2       1       3       3       1       1 
CND_881 CND_882 CND_883 CND_884 CND_885 CND_886 CND_887 CND_888 
CND_889 CND_890 CND_891 CND_892 CND_893 CND_894 CND_895 CND_896 
      1       1       1       1       1       1       1       1       1       1       1       1       1       1       3       1 
CND_897 CND_898 CND_899 CND_900 CND_901 CND_902 CND_903 CND_904 
CND_905 CND_906 CND_907 CND_908 CND_909 CND_910 CND_911 CND_912 
      1       1       1       1       1       3       1       1       1       1       1       1       1       1       1       1 
CND_913 CND_914 CND_915 CND_916 CND_917 CND_918 CND_919 CND_920 
CND_921 CND_922 CND_923 CND_924 CND_925 CND_926 CND_927 CND_928 
      1       1       2       2       1       1       1       1       1       1       1       1       1       2       1       1 
CND_929 CND_930 CND_931 
      1       2       1 
```

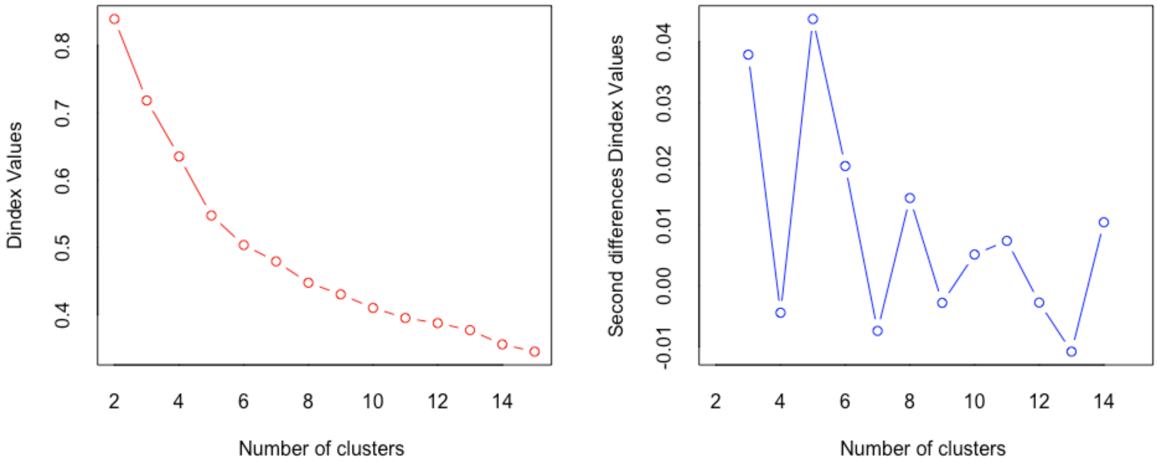


Figure F-17: Hierarchical clustering of dentine isotope data D-index outputs for optimal clusters.

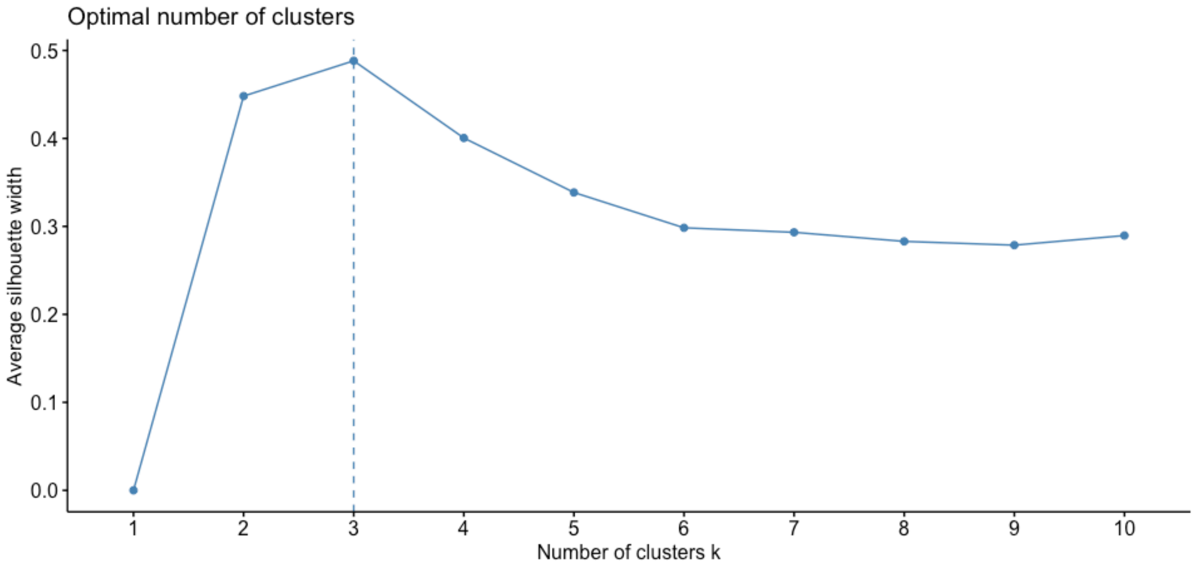


Figure F-18: Silhouette method for optimal number of hierarchical clusters for bone $\delta^{13}C$ and $\delta^{15}N$.

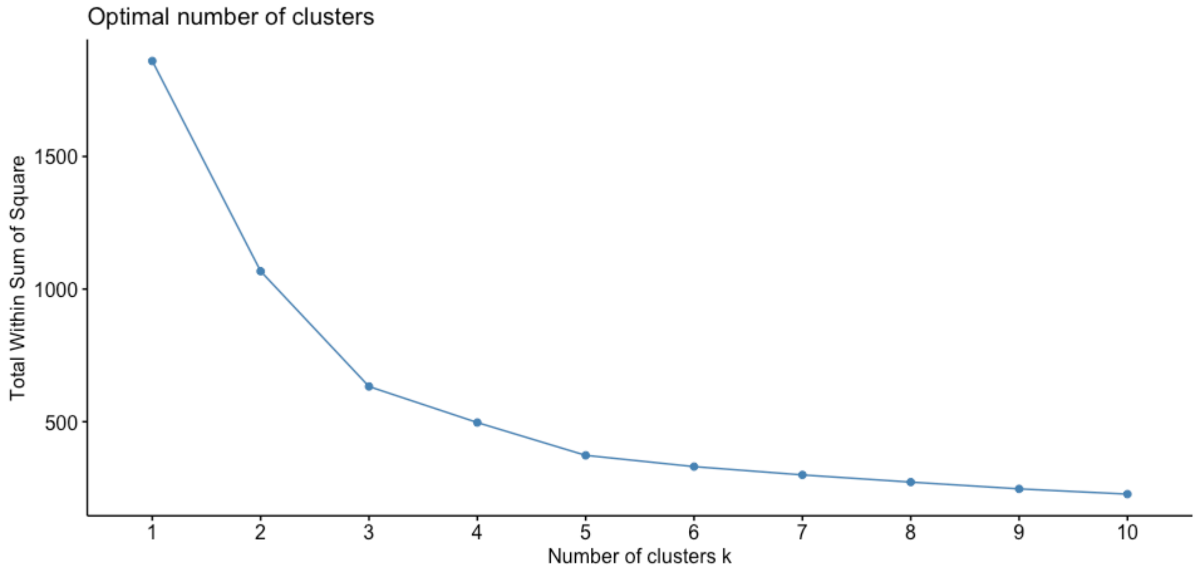


Figure F-19: Elbow method for optimal number of hierarchical clusters for bone δ13C and δ15N.

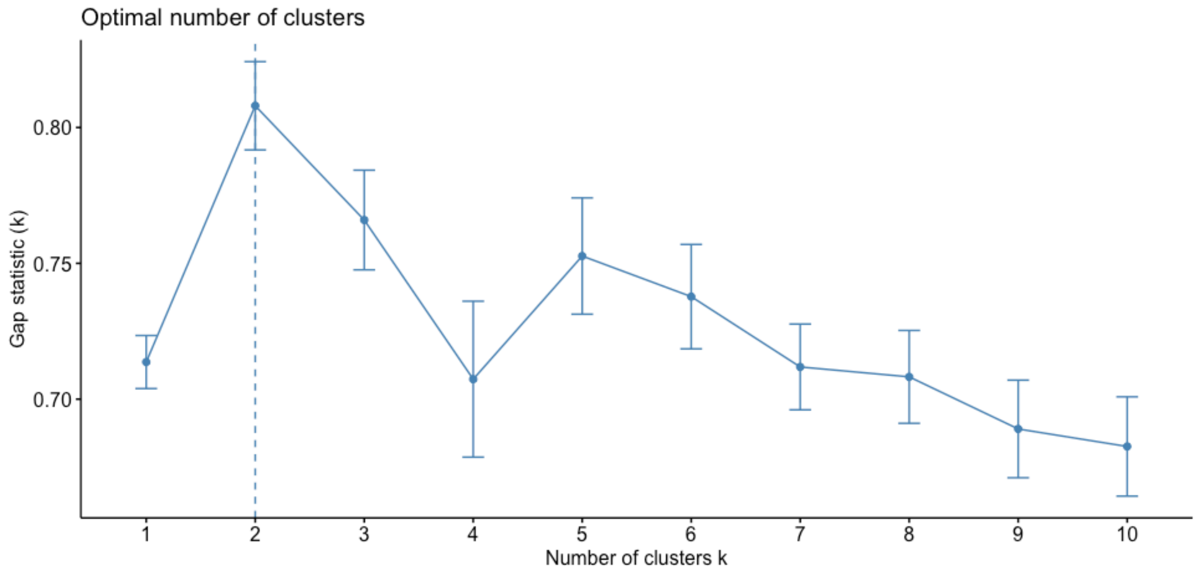


Figure F-20: Gap statistic method for optimal number of hierarchical clusters for bone δ13C and δ15N.

G DetectingDeviatingCells Outputs

G.i DDC Algorithm Details and Outputs for all of Kent

The input data has 237 rows and 24 columns.

The input data contained 9 non-numeric columns (variables).
Their column names are:

[1] ID Site date_cat age_cat grave_orientation body_position
internment_style bone_sampled
[9] tooth_sampled

These columns will be ignored in the analysis.
We continue with the remaining 15 numeric columns:

[1] stature_cm num_ggoods num_foreign_ggoods
grave_orientation_degrees bone_d13C
[6] bone_d15N dentine_d13C dentine_d15N enamel_d13C
enamel_d18O_chenery
[11] DELTA13C_dent_bone DELTA15N_dent_bone DELTA13C_enamel_dent
DELTA18O_dwMAP Church_distance

The data contained 140 rows with over 50% of NAs.
Their row names are:

[1] FING_16 FING_106 FING_118 FING_133
[5] FING_168 FING_179 GrN-30967 GrN-30968
[9] GrN-30969 GrN-30970 GrN-30971 GrN-30972
[13] GrN-30973 SUERC-40306 SUERC-40307 SUERC-
40308
[17] SPT_8 SPT_42 SPT_68 SPT_113
[21] SPT_194 SPT_196 SPT_212 SPT_250
[25] SPT_263 SPT_318 SPT_360 SPT_205(208??)
[29] POL10 POL100 POL102N POL102S
[33] POL2 POL36 POL38 POL39
[37] POL4 POL40 POL41 POL42N
[41] POL42S POL43N POL43S POL44
[45] POL45 POL46 POL47 POL5
[49] POL52N POL52S POL53 POL56
[53] POL57 POL60L POL60U POL61
[57] POL62 POL64N POL64S POL65
[61] POL67 POL68(N) POL68S POL69N
[65] POL69S POL71 POL72 POL73
[69] POL75N POL75S POL76 POL77
[73] POL81N POL82N POL82S POL83
[77] POL84 POL85 POL86N POL86S
[81] POL87 POL88 POL89 POL90
[85] POL91 POL92 POL93 POL95N
[89] POL97 POL98 POL99C POL99N
[93] POL99S GH_Primary burial (burial 24?) LYM_1672
DBC94_222

[97] DBC94_391A DBC94_339 DBC94_414 HOLB_17
[101] HOLB_18.2 HOLB_29 HOLB_33 HOLB_35
[105] HOLB_36 SRD88_35 SRD88_71 SRD88_81
[109] SRD88_86 SRD88_95 SRD88_100 SRD88_40
[113] SRD88_64 SRD88_68 SRD88_79 CEF_2839
[117] EAST_52 EAST_1056-1057 EAST_4 EAST_63
[121] EAST_66 EAST_110 EAST_156 EAST_189
[125] EAST_232 EAST_263 EAST_269 EAST_308
[129] EAST_354 EAST_380 EAST_472 EAST_649
[133] EAST_680 EAST_752 EAST_795 RING-18
[137] RING-25 RING-30 RING-40 RING-41

These rows will be ignored in the analysis.
We continue with the remaining 97 rows:

[1] FING_6 FING_8 FING_15 FING_18 FING_21A FING_21B FING_26A
FING_30 FING_47B FING_48 FING_57 FING_61 FING_62B
[14] FING_63 FING_64 FING_72 FING_73 FING_82 FING_84 FING_105
FING_113 FING_116 FING_121 FING_123 FING_124 FING_125A
[27] FING_129A FING_129B FING_135 FING_138 FING_144 FING_145A FING_150
FING_158 FING_165 FING_175 FING_180 FING_193 FING_199
[40] FING_208 RING-8 RING-39 NC 2611 DBC92_204 DBC94_250 DBC94_264
DBC94_271 DBC94_297 DBC94_323 DBC94_336 DBC94_346 DBC94_347
[53] DBC94_375 DBC94_407 DBC94_420 DBC94_391B DBC94_426 HOLB_8
HOLB_13 HOLB_15 HOLB_18.1 HOLB_19 HOLB_21 HOLB_23 HOLB_24
[66] HOLB_25 HOLB_28 HOLB_30 HOLB_32 HOLB_37 HOLB_5 HOLB_20
HOLB_27 SRD88_17 SRD88_22 SRD88_34 SRD88_57 SRD88_75
[79] SRD88_83 SRD88_84 SRD88_90 SRD88_93 SRD88_98 SRD88_104
SRD88_106 SRD88_105A SRD88_105B SRD88_105C SRD88_25A SRD88_25B
SRD88_94
[92] SRD88_73A SRD87_33 SRD88_76 SRD88_80 SRD88_82 SRD88_89

The data contained 1 columns with over 50% of NAs.
Their column names are:

[1] stature_cm

These columns will be ignored in the analysis.
We continue with the remaining 14 columns:

[1] num_ggoods num_foreign_ggoods grave_orientation_degrees
bone_d13C bone_d15N
[6] dentine_d13C dentine_d15N enamel_d13C
enamel_d18O_chenery DELTA13C_dent_bone
[11] DELTA15N_dent_bone DELTA13C_enamel_dent DELTA18O_dwMAP
Church_distance

The data contained 1 columns with zero or tiny median absolute deviation.
Their column names are:

[1] num_foreign_ggoods

These columns will be ignored in the analysis.
We continue with the remaining 13 columns:

[1] num_ggoods grave_orientation_degrees bone_d13C bone_d15N
dentine_d13C
[6] dentine_d15N enamel_d13C enamel_d18O_chenery
DELTA13C_dent_bone DELTA15N_dent_bone
[11] DELTA13C_enamel_dent DELTA18O_dwMAP Church_distance

The final data set we will analyze has 97 rows and 13 columns.

G.ii DDC Algorithm Details and Outputs for all of Kent – dietary only

The input data has 237 rows and 22 columns.

The input data contained 9 non-numeric columns (variables).
Their column names are:

[1] ID Site date_cat age_cat grave_orientation body_position
internment_style bone_sampled
[9] tooth_sampled

These columns will be ignored in the analysis.
We continue with the remaining 13 numeric columns:

[1] stature_cm num_ggoods num_foreign_ggoods
grave_orientation_degrees bone_d13C
[6] bone_d15N dentine_d13C dentine_d15N enamel_d13C
DELTA13C_dent_bone
[11] DELTA15N_dent_bone DELTA13C_enamel_dent Church_distance

The data contained 75 rows with over 50% of NAs.
Their row names are:

[1] FING_16 GrN-30968 GrN-30970 SUERC-40306
[5] SUERC-40307 SUERC-40308 SPT_8 SPT_42
[9] SPT_68 SPT_113 SPT_194 SPT_196
[13] SPT_212 SPT_250 SPT_263 SPT_318
[17] SPT_360 SPT_205(208??) POL10 POL2
[21] POL36 POL4 POL5 POL64S
[25] POL72 POL83 POL86N RING-8
[29] RING-39 GH_Primary burial (burial 24?) LYM_1672
DBC94_222
[33] DBC94_391A DBC94_339 DBC94_414 HOLB_17
[37] HOLB_18.2 HOLB_29 HOLB_33 HOLB_35
[41] HOLB_36 SRD88_35 SRD88_71 SRD88_81
[45] SRD88_86 SRD88_100 SRD88_40 SRD88_64
[49] SRD88_68 SRD88_79 CEF_2839 EAST_52
[53] EAST_1056-1057 EAST_4 EAST_63 EAST_66

[57] EAST_110 EAST_156 EAST_189 EAST_232
[61] EAST_263 EAST_269 EAST_308 EAST_354
[65] EAST_380 EAST_472 EAST_649 EAST_680
[69] EAST_752 EAST_795 RING-18 RING-25
[73] RING-30 RING-40 RING-41

These rows will be ignored in the analysis.
We continue with the remaining 162 rows:

[1] FING_6 FING_8 FING_15 FING_18 FING_21A FING_21B FING_26A
FING_30 FING_47B FING_48 FING_57 FING_61 FING_62B
[14] FING_63 FING_64 FING_72 FING_73 FING_82 FING_84 FING_105
FING_106 FING_113 FING_116 FING_118 FING_121 FING_123
[27] FING_124 FING_125A FING_129A FING_129B FING_133 FING_135 FING_138
FING_144 FING_145A FING_150 FING_158 FING_165 FING_168
[40] FING_175 FING_179 FING_180 FING_193 FING_199 FING_208 GrN-30967
GrN-30969 GrN-30971 GrN-30972 GrN-30973 POL100 POL102N
[53] POL102S POL38 POL39 POL40 POL41 POL42N POL42S POL43N
POL43S POL44 POL45 POL46 POL47
[66] POL52N POL52S POL53 POL56 POL57 POL60L POL60U POL61
POL62 POL64N POL65 POL67 POL68(N)
[79] POL68S POL69N POL69S POL71 POL73 POL75N POL75S POL76
POL77 POL81N POL82N POL82S POL84
[92] POL85 POL86S POL87 POL88 POL89 POL90 POL91 POL92
POL93 POL95N POL97 POL98 POL99C
[105] POL99N POL99S NC 2611 DBC92_204 DBC94_250 DBC94_264
DBC94_271 DBC94_297 DBC94_323 DBC94_336 DBC94_346 DBC94_347
DBC94_375
[118] DBC94_407 DBC94_420 DBC94_391B DBC94_426 HOLB_8 HOLB_13
HOLB_15 HOLB_18.1 HOLB_19 HOLB_21 HOLB_23 HOLB_24 HOLB_25
[131] HOLB_28 HOLB_30 HOLB_32 HOLB_37 HOLB_5 HOLB_20 HOLB_27
SRD88_17 SRD88_22 SRD88_34 SRD88_57 SRD88_75 SRD88_83
[144] SRD88_84 SRD88_90 SRD88_93 SRD88_95 SRD88_98 SRD88_104
SRD88_106 SRD88_105A SRD88_105B SRD88_105C SRD88_25A SRD88_25B
SRD88_94
[157] SRD88_73A SRD87_33 SRD88_76 SRD88_80 SRD88_82 SRD88_89

The data contained 1 columns with zero or tiny median absolute deviation.
Their column names are:

[1] num_foreign_ggoods

These columns will be ignored in the analysis.
We continue with the remaining 12 columns:

[1] stature_cm num_ggoods grave_orientation_degrees bone_d13C
bone_d15N
[6] dentine_d13C dentine_d15N enamel_d13C
DELTA13C_dent_bone DELTA15N_dent_bone
[11] DELTA13C_enamel_dent Church_distance

The final data set we will analyze has 162 rows and 12 columns.

G.iii DDC Algorithm Details and Outputs for all of Kent – mobility only

The input data has 237 rows and 16 columns.

The input data contained 9 non-numeric columns (variables).
Their column names are:

[1] ID Site date_cat age_cat grave_orientation body_position
internment_style bone_sampled
[9] tooth_sampled

These columns will be ignored in the analysis.
We continue with the remaining 7 numeric columns:

[1] stature_cm num_ggoods num_foreign_ggoods
grave_orientation_degrees enamel_d18O_chenery
[6] DELTA18O_dwMAP Church_distance

The data contained 15 rows with over 50% of NAs.
Their row names are:

[1] SPT_8 SPT_42 SPT_68 SPT_113 SPT_194 SPT_196 SPT_212
SPT_250 SPT_263
[10] SPT_318 SPT_360 SPT_205(208??) POL2 LYM_1672 CEF_2839

These rows will be ignored in the analysis.
We continue with the remaining 222 rows:

[1] FING_6 FING_8 FING_15 FING_16
[5] FING_18 FING_21A FING_21B FING_26A
[9] FING_30 FING_47B FING_48 FING_57
[13] FING_61 FING_62B FING_63 FING_64
[17] FING_72 FING_73 FING_82 FING_84
[21] FING_105 FING_106 FING_113 FING_116
[25] FING_118 FING_121 FING_123 FING_124
[29] FING_125A FING_129A FING_129B FING_133
[33] FING_135 FING_138 FING_144 FING_145A
[37] FING_150 FING_158 FING_165 FING_168
[41] FING_175 FING_179 FING_180 FING_193
[45] FING_199 FING_208 GrN-30967 GrN-30968
[49] GrN-30969 GrN-30970 GrN-30971 GrN-30972
[53] GrN-30973 SUERC-40306 SUERC-40307 SUERC-
40308
[57] POL10 POL100 POL102N POL102S
[61] POL36 POL38 POL39 POL4
[65] POL40 POL41 POL42N POL42S
[69] POL43N POL43S POL44 POL45
[73] POL46 POL47 POL5 POL52N

```
 [77] POL52S             POL53              POL56              POL57
 [81] POL60L             POL60U             POL61              POL62
 [85] POL64N             POL64S             POL65              POL67
 [89] POL68(N)           POL68S             POL69N             POL69S
 [93] POL71              POL72              POL73              POL75N
 [97] POL75S             POL76              POL77              POL81N
[101] POL82N             POL82S             POL83              POL84
[105] POL85              POL86N             POL86S             POL87
[109] POL88              POL89              POL90              POL91
[113] POL92              POL93              POL95N             POL97
[117] POL98              POL99C             POL99N             POL99S
[121] RING-8             RING-39            GH_Primary burial (burial 24?) NC 
2611
[125] DBC92_204          DBC94_222          DBC94_250          DBC94_264
[129] DBC94_271          DBC94_297          DBC94_323          DBC94_336
[133] DBC94_346          DBC94_347          DBC94_375          DBC94_407
[137] DBC94_420          DBC94_391A         DBC94_391B 
DBC94_426
[141] DBC94_339          DBC94_414          HOLB_8             HOLB_13
[145] HOLB_15            HOLB_17            HOLB_18.1          HOLB_18.2
[149] HOLB_19            HOLB_21            HOLB_23            HOLB_24
[153] HOLB_25            HOLB_28            HOLB_29            HOLB_30
[157] HOLB_32            HOLB_33            HOLB_35            HOLB_36
[161] HOLB_37            HOLB_5             HOLB_20            HOLB_27
[165] SRD88_17           SRD88_22           SRD88_34           SRD88_35
[169] SRD88_57           SRD88_71           SRD88_75           SRD88_81
[173] SRD88_83           SRD88_84           SRD88_86           SRD88_90
[177] SRD88_93           SRD88_95           SRD88_98           SRD88_100
[181] SRD88_104          SRD88_106          SRD88_105A 
SRD88_105B
[185] SRD88_105C         SRD88_25A          SRD88_25B          SRD88_40
[189] SRD88_64           SRD88_68           SRD88_79           SRD88_94
[193] SRD88_73A          SRD87_33           SRD88_76           SRD88_80
[197] SRD88_82           SRD88_89           EAST_52            EAST_1056-
1057
[201] EAST_4             EAST_63            EAST_66            EAST_110
[205] EAST_156           EAST_189           EAST_232           EAST_263
[209] EAST_269           EAST_308           EAST_354           EAST_380
[213] EAST_472           EAST_649           EAST_680           EAST_752
[217] EAST_795           RING-18            RING-25            RING-30
[221] RING-40            RING-41
```

The data contained 1 columns with zero or tiny median absolute deviation.
Their column names are:

[1] num_foreign_ggoods

These columns will be ignored in the analysis.
We continue with the remaining 6 columns:

[1] stature_cm num_ggoods grave_orientation_degrees
enamel_d18O_chenery DELTA18O_dwMAP
[6] Church_distance

The final data set we will analyze has 222 rows and 6 columns.

G.iv DDC Algorithm Details and Outputs for Finglesham

The input data has 46 rows and 27 columns.

The input data contained 10 non-numeric columns (variables).
Their column names are:

[1] ID date_cat age_cat grave_orientation body_position
internment_style
[7] bone_sampled tooth_sampled O_Sr_C_cluster O_Sr_cluster

These columns will be ignored in the analysis.
We continue with the remaining 17 numeric columns:

[1] stature_cm num_ggoods num_foreign_ggoods
grave_orientation_degrees
[5] bone_d13C bone_d15N dentine_d13C dentine_d15N
[9] enamel_d13C enamel_d18O_chenery DELTA13C_dent_bone
DELTA15N_dent_bone
[13] DELTA13C_enamel_dent DELTA18O_dwMAP O_C_cluster
CNB_cluster
[17] CND_cluster

The data contained 6 rows with over 50% of NAs.
Their row names are:

[1] FING_16 FING_106 FING_118 FING_133 FING_168 FING_179

These rows will be ignored in the analysis.
We continue with the remaining 40 rows:

[1] FING_6 FING_8 FING_15 FING_18 FING_21A FING_21B FING_26A FING_30
FING_47B FING_48 FING_57 FING_61
[13] FING_62B FING_63 FING_64 FING_72 FING_73 FING_82 FING_84 FING_105
FING_113 FING_116 FING_121 FING_123
[25] FING_124 FING_125A FING_129A FING_129B FING_135 FING_138 FING_144
FING_145A FING_150 FING_158 FING_165 FING_175
[37] FING_180 FING_193 FING_199 FING_208

The data contained 4 discrete columns with 3 or fewer values.
Their column names are:

[1] num_foreign_ggoods O_C_cluster CNB_cluster CND_cluster

These columns will be ignored in the analysis.

We continue with the remaining 13 columns:

```
 [1] stature_cm              num_ggoods              grave_orientation_degrees bone_d13C
 [5] bone_d15N               dentine_d13C            dentine_d15N              enamel_d13C
 [9] enamel_d18O_chenery     DELTA13C_dent_bone      DELTA15N_dent_bone
DELTA13C_enamel_dent
[13] DELTA18O_dwMAP
```

The final data set we will analyze has 40 rows and 13 columns.

H Height/Stature and Dietary Isotopes

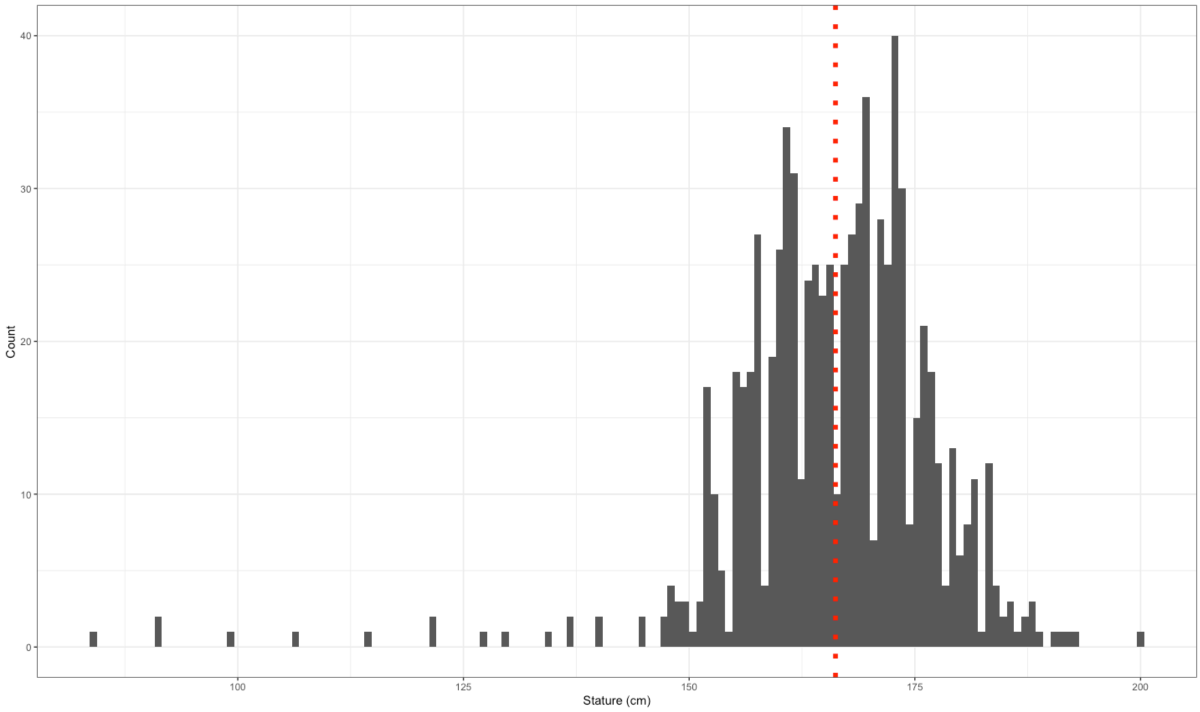


Figure H-1: Histogram of stature (cm) in Early Medieval England, red dotted line indicates mean value.

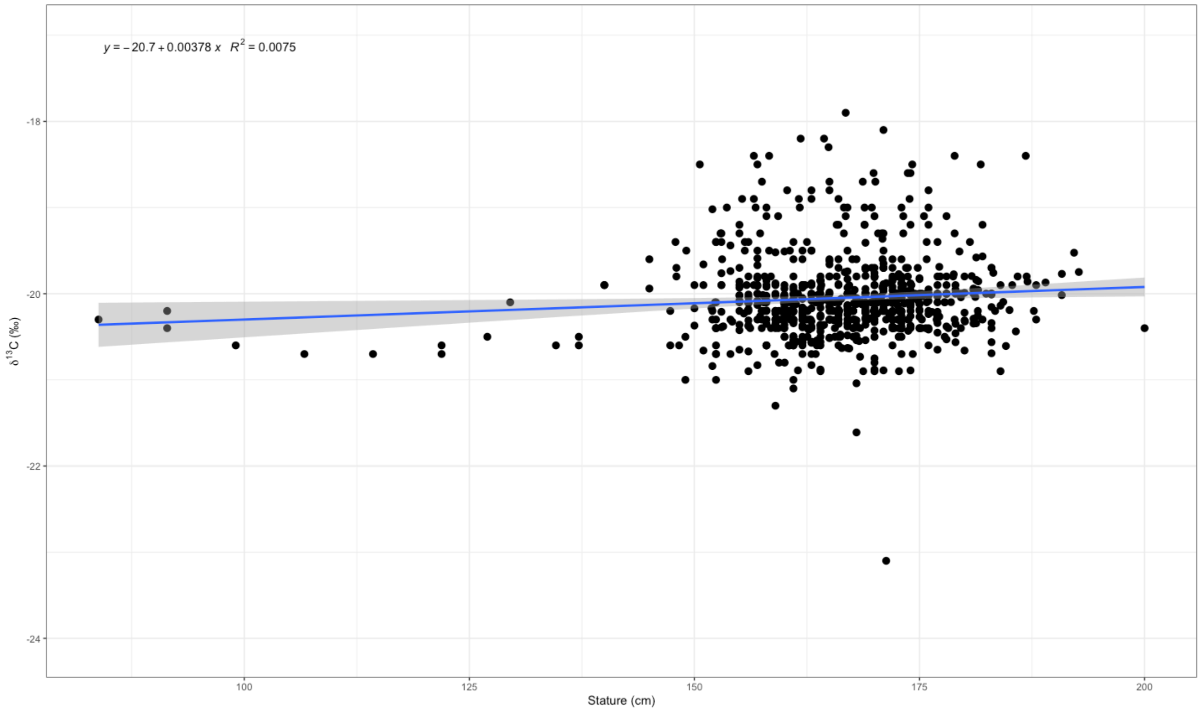


Figure H-2: Scatterplot with overlaid linear model of stature (cm) and δ13C bone values from Early Medieval England, $y=-20.7 + 0.00378x$ $R^2= 0.0075$.

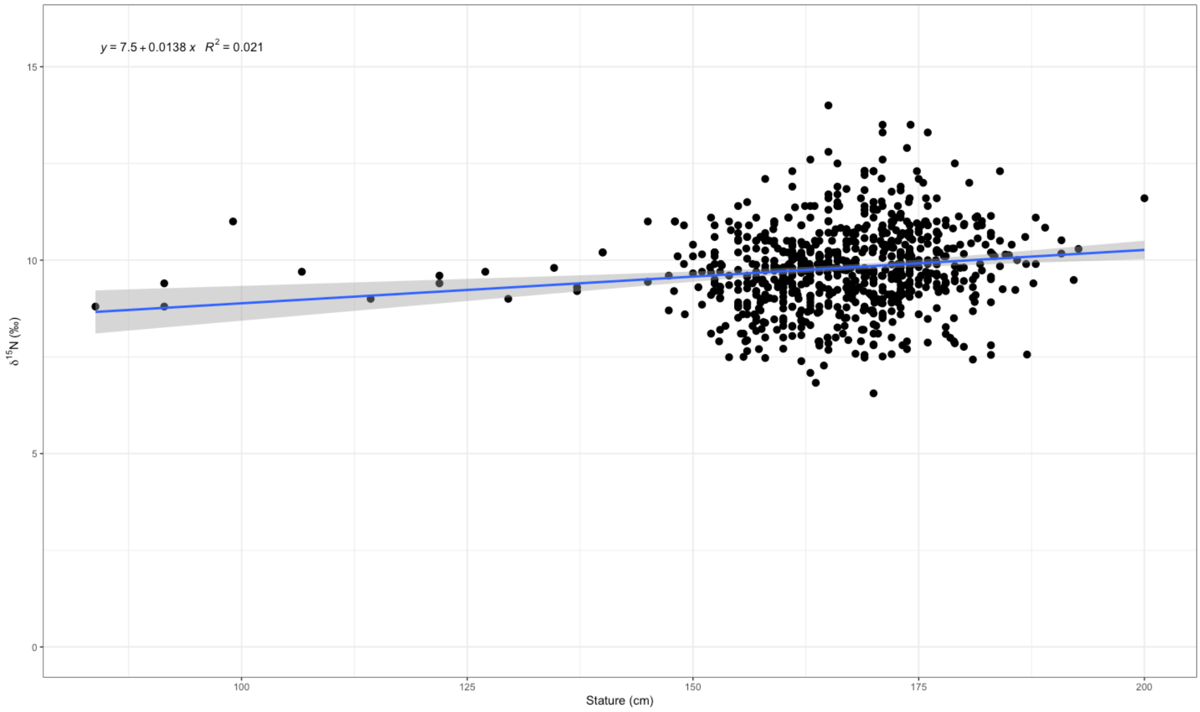


Figure H-3: Scatterplot with overlaid linear model of stature (cm) and δ15N bone values from Early Medieval England, y=7.5 + 0.0138x R^2= 0.021.

I Diet and Age Categories Ungrouped

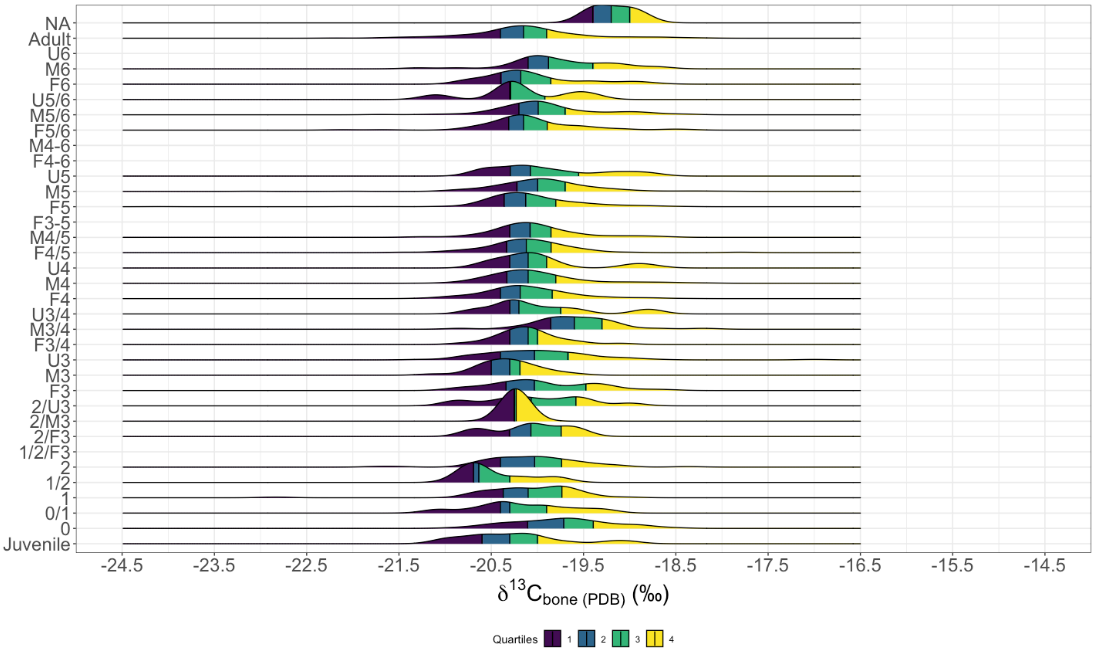


Figure I-1: Ridge plot of bone $\delta^{13}C_{coll}$ values from England by gendered age categories (see Chapter 3 for age ranges).

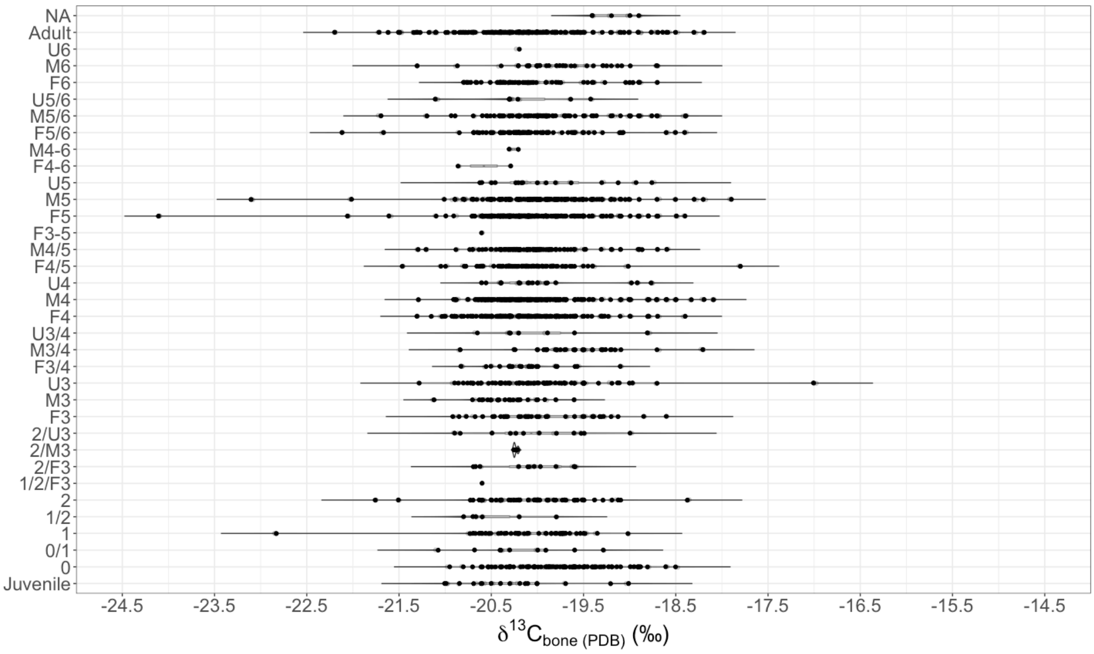


Figure I-2: Violin plot of bone $\delta^{13}C_{coll}$ values from England by gendered age categories (see Chapter 3 for age ranges).

The age categories in these figures are in their rawest form with many individuals straddling two age categories, and as such sample sizes are not ideal in some categories. However, what these do show is good alignment of the ranges and quartiles for the majority of age categories for both bone $\delta^{13}C_{coll}$ and $\delta^{15}N_{coll}$ values.

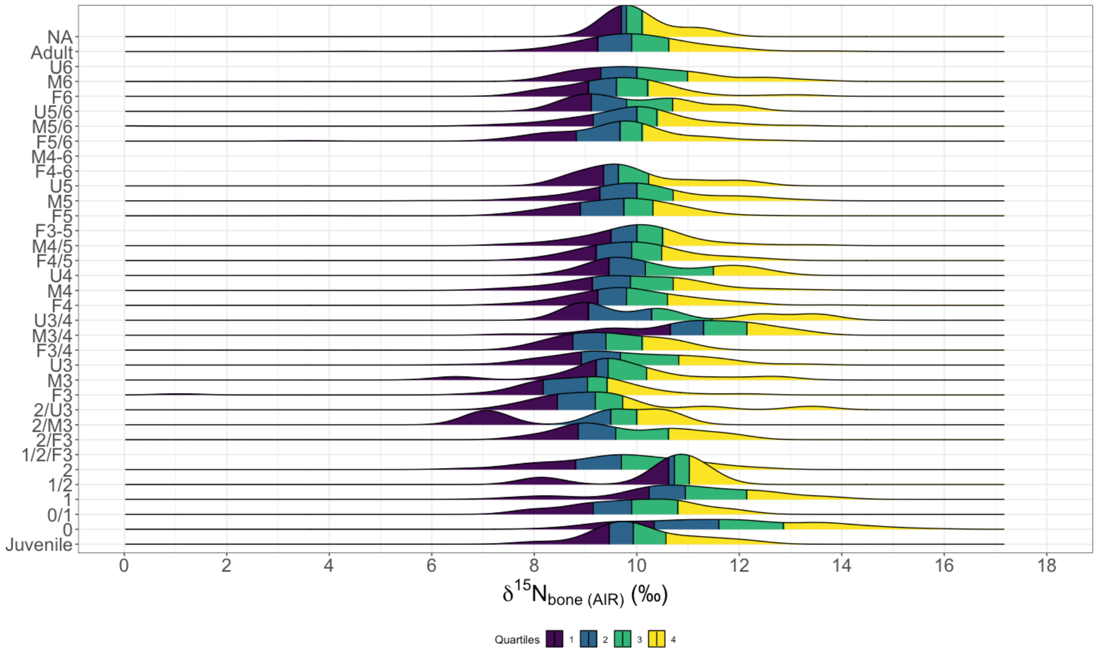


Figure I-3: Ridge plot of bone $\delta^{15}N_{coll}$ values from England by gendered age categories (see Chapter 3 for age ranges).

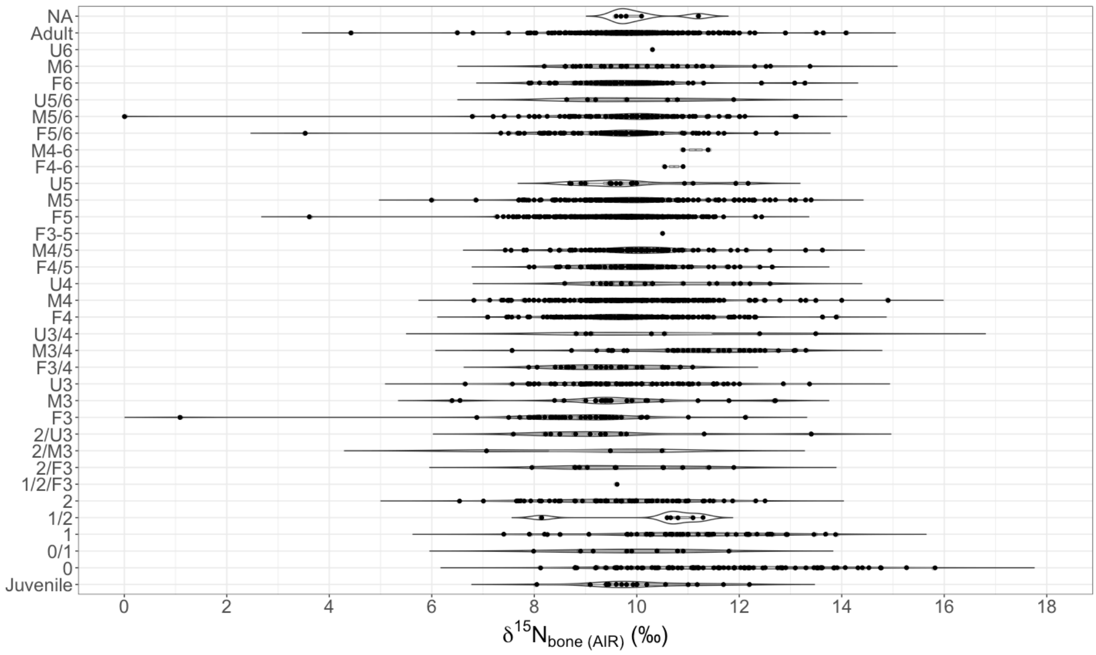


Figure I-4: Violin plot of bone $\delta^{15}N_{coll}$ values from England by gendered age categories (see Chapter 3 for age ranges).

J Social Status, Burial Provision and Diet

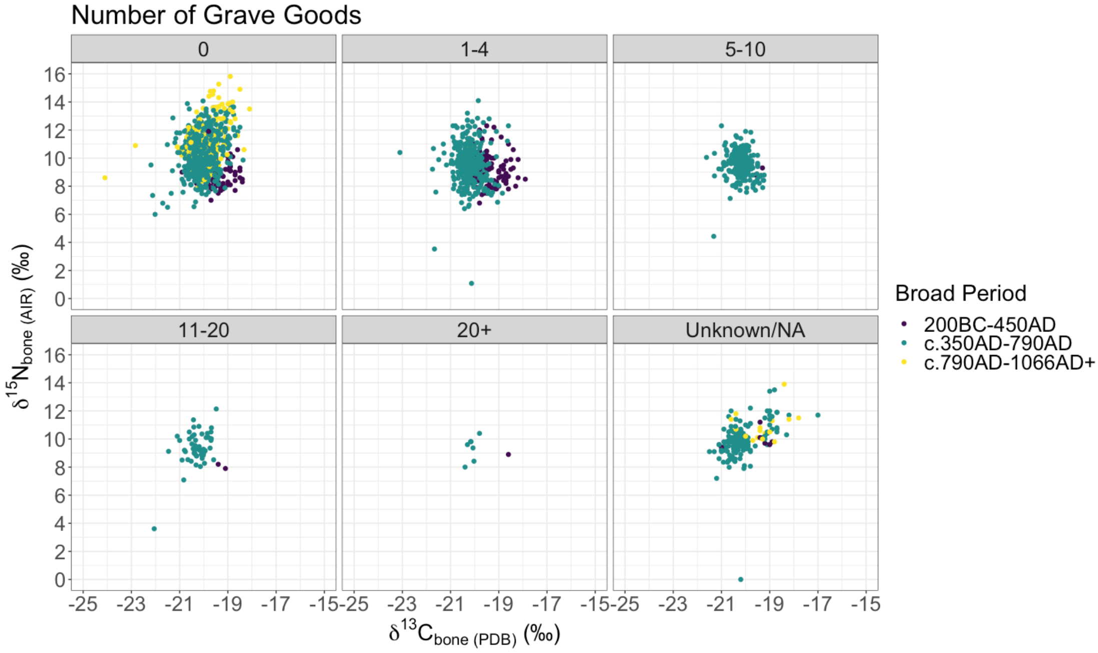


Figure J-1: Scatterplots of human bone $\delta^{13}C_{coll}$ and $\delta^{15}N_{coll}$ values by number of grave goods, coloured by time period.

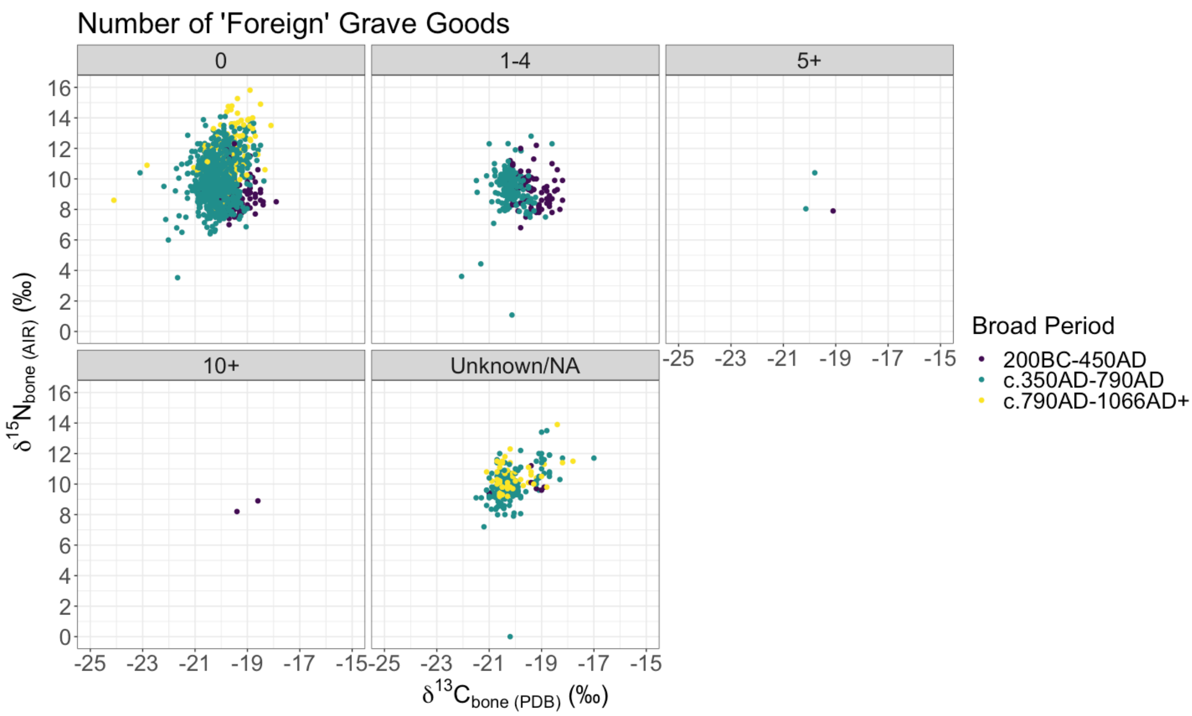


Figure J-2: Scatterplots of human bone $\delta^{13}C_{coll}$ and $\delta^{15}N_{coll}$ values by number of 'foreign' grave goods, coloured by time period.

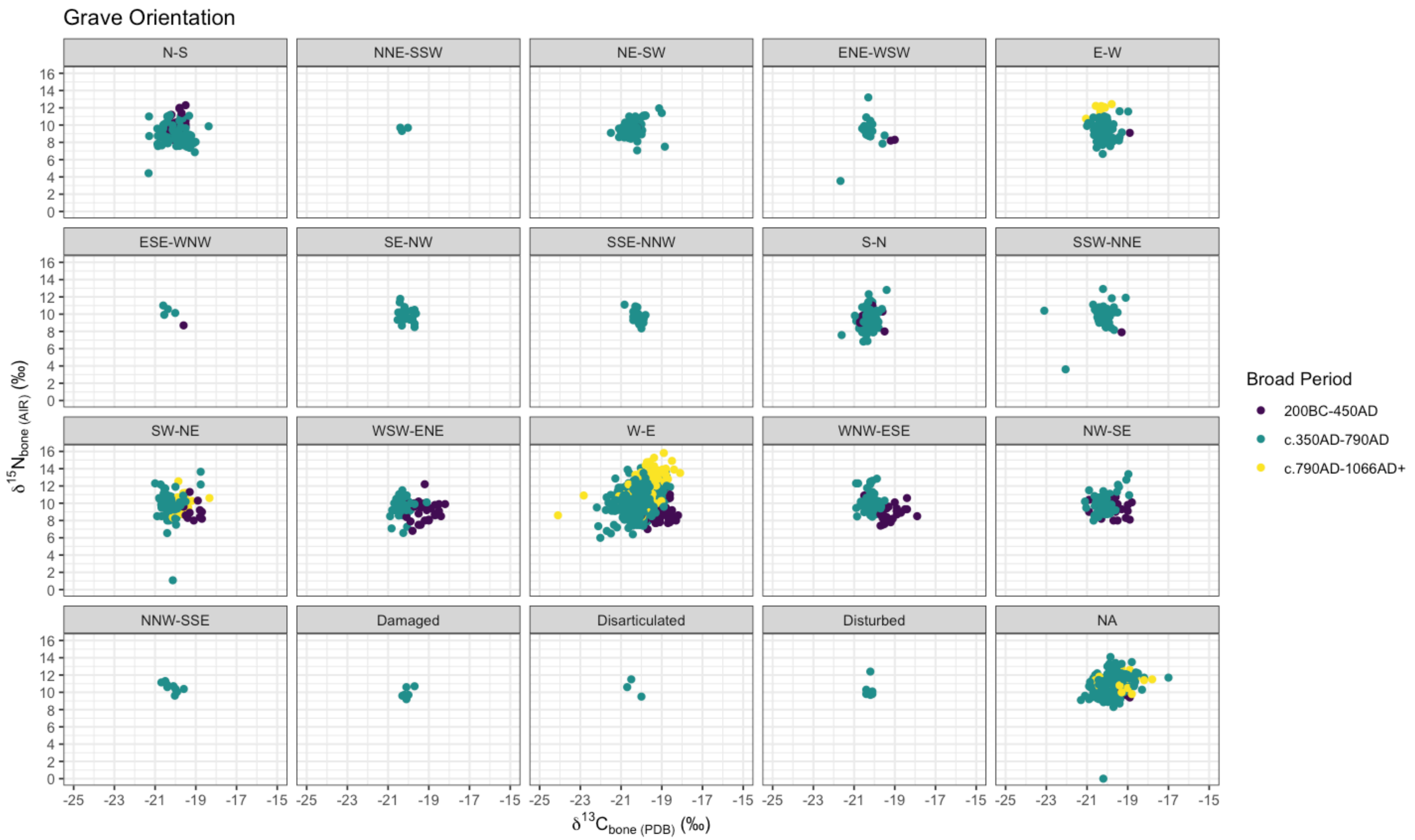


Figure J-3: Scatterplots of human bone $\delta^{13}C_{coll}$ and $\delta^{15}N_{coll}$ values by grave orientation, coloured by time period.

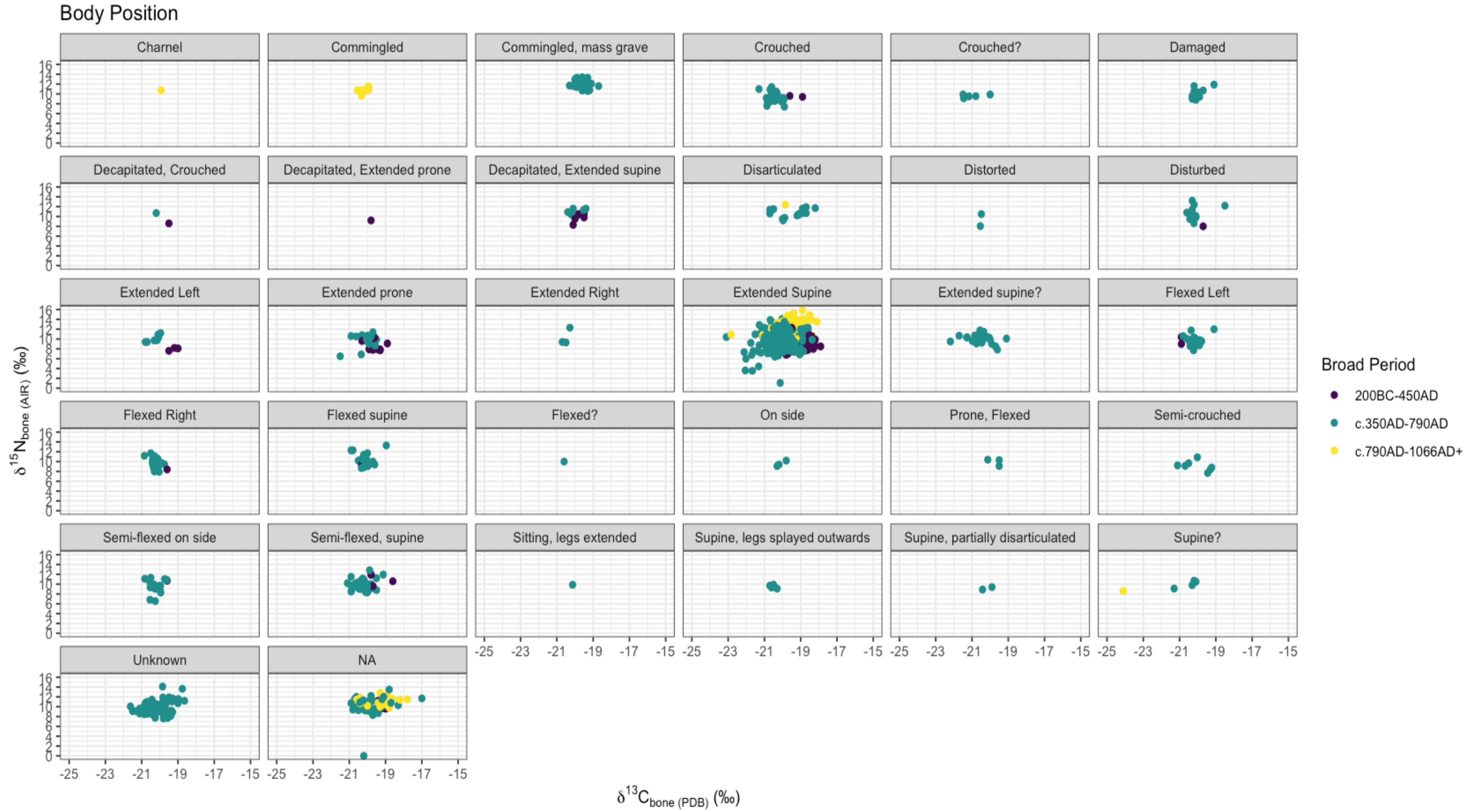


Figure J-4: Scatterplots of human bone $\delta^{13}C_{coll}$ and $\delta^{15}N_{coll}$ values by body position, coloured by time period.

K Hines et al. (2013: 460) Grave Good Chronological Phases

Male Phases from Correspondence Analysis	**Date Ranges**
p – AS-Mp	AD 525-570
q – AS-Mq	AD 550-595
r – AS-Mr	AD 565-615
s – AS-Ms	AD 585-645
t – AS-Mt	AD 610-685
Male Phases from Leading Artefact Typologies	
a – AS-MB	AD 525-565
b – AS-MC	AD 545-595
c – AS-MD	AD 565-610
d – AS-ME	AD 580-645
e – AS-MF	AD 610-685
Female Phases from Leading Artefact Typologies	
a – AS-FB	AD 510-585
b – AS-FC	AD 555-640
c – AS-FD	AD 580-650
d – AS-FE	AD 625-680

Table K-1 – Male and Female grave good chronological phases from Hines et al. (2013, 460).