Supplemental Material

Early formation and taphonomic significance of kaolinite associated with Burgess Shale fossils

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1. Supplemental methodological details

1.1. Specimen Details
All specimens are housed in the National Museum of Natural History, Smithsonian Institution, Washington DC, USA (USNM). Specimens derive from the Phyllopod Bed of the classic Burgess Shale Walcott Quarry (middle Cambrian Wuliuan Stage, Burgess Shale Formation, British Columbia, Canada), possibly the best of the Burgess Shale-type (BST) deposits in terms of preservation (Saleh et al., 2020). Fossils were selected to enable X-ray diffraction (XRD) analysis: The specimen was as flat as possible and small enough to enable mounting in the diffractometer. Where part and counterpart are available, analyses were taken from both and combined. Figs. S1–S15 show areas where selected-area XRD was performed. Areas were classified as either fossil or matrix. If any part of an analyzed area overlapped with the fossil, the area was classified as fossil.

| Specimen          | USNM PAL | Part/Counterpart | Reference                          |
|-------------------|----------|------------------|-----------------------------------|
| Canadia spinosa   | USNM PAL | 198723           | Pl. 3 Fig. 38: Conway Morris, 1979 |
| Canadia spinosa   | USNM PAL | 198724           | Pl. 3 Fig. 37: Conway Morris, 1979 |
| Canadia spinosa   | USNM PAL | 199758           | Pl. 3 Fig. 38, 40: Conway Morris, 1979 |
| Marrella splendens| USNM PAL | 166587           | Pl. 11 Fig. 3: Whittington, 1971   |
| Marrella splendens| USNM PAL | 229990           | Not figured                       |
| Marrella splendens| USNM PAL | 230379           | Not figured                       |
| Opabinia regalis  | USNM PAL | 139217           | Pl. 5 Fig. 25, 26: Whittington, 1975 |
| Opabinia regalis  | USNM PAL | 155600           | Pl. 7 Fig. 37, Pl. 8 Fig. 41–45: Whittington, 1975 |
| Ottoia prolifica  | USNM PAL | 188616           | Pl. 2 Fig. 7: Conway Morris, 1977  |
| Ottoia prolifica  | USNM PAL | 188617           | Pl. 2 Fig. 4: Conway Morris, 1977  |
| Ottoia prolifica  | USNM PAL | 198565           | Pl. 2 Fig. 3: Conway Morris, 1977  |
| Ottoia prolifica  | USNM PAL | 198577           | Pl. 10 Fig. 1: Conway Morris, 1977 |
| Pikaia gracilens  | USNM PAL | 198688           | Fig. 5A, 11C, D: Conway Morris and Caron, 2012 |
| Pikaia gracilens  | USNM PAL | 198692           | Fig. 9A: Conway Morris and Caron, 2012 |
| Pikaia gracilens  | USNM PAL | 202220           | Fig. 12A–C: Conway Morris and Caron, 2012 |

Orr et al. (1998) noted that aluminum is concentrated in the digestive systems of Marrella. To corroborate this observation and to identify the mineral host of any aluminum enrichment, areas analyzed by selected-area XRD that overlapped with the digestive system were noted. Anatomy was identified based on published descriptions: Canadia (Conway Morris, 1979; Parry and Caron, 2019), Marrella (Whittington, 1971), Opabinia (Whittington, 1975; Zhang and Briggs, 2007), Ottoia (Conway Morris, 1977), Pikaia (Conway Morris and Caron, 2012).

1.2. Selected-Area XRD

System set-up
Selected-area XRD was performed on a PANalytical Empyrean diffractometer, employing a Co Kα source and PIXcel-1D detector, at the Department of Earth Sciences, University of Oxford, UK. In all cases the length of sample irradiated by X-rays was kept at a constant value of 1 mm using a programmable divergence slit and 0.25° anti-scatter slit. Employing a 5 mm beam mask gave an irradiated width of 7 mm, while a 10 mm mask gave a width of 12 mm, and a 20 mm mask gave a width of 22 mm (length and width refer to the orientation of the diffractometer). Thus, select areas measuring 7×1, 12×1, and 22×1 mm could be analyzed. Areas 7×1 mm were preferred, but the size of some specimens, e.g., Opabinia, dictated larger areas in order to access
some anatomical features. Even though these configurations constrained the geometry of the irradiated area, the dimensions and precise position of the irradiated area required visual verification. This was performed using a flat phosphor plate that fluoresces upon X-ray irradiation. X-ray penetration is dependent on substrate but is likely to be on the order of 100 µm.

**Data acquired**

Data were collected from selected areas over 5–80° 2θ in 0.0263° steps numbering 2856, with a total collection time for each selected area of ~5 hours.

**Mineral identification – Highscore Data**

Minerals were identified and their relative abundance quantified using the reference intensity ratio method (Snyder and Bish, 1989) with PANalytical Highscore software (https://www.malvernanalytical.com/en/products/category/software/x-ray-diffraction-software/highscore) and the Powder Diffraction File-4+ database (International Center for Diffraction Data: http://www.icdd.com/pdf-4/). These data are referred to here as “Highscore data”. Prior to mineral identification, intensities were transformed to those corresponding to collection via a fixed divergence slit, and the background of each diffraction pattern was subtracted. If trace amounts of a mineral were identified, its relative abundance was listed as 0.5%. Rounding of relative abundances occasionally meant that the total for a given sample was slightly lower/higher than 100%.

**Mineral identification – Fityk Data**

Since precise identification of individual clay minerals is difficult using the Highscore data, the ~7 Å peak was analyzed to confirm identifications. Both kaolinite and chlorite have peaks in the vicinity of ~7 Å (Kaolinite ~7.15 Å, Chlorite 7.08–7.14 Å; Moore and Reynolds, 1997). To ensure precise kaolinite identification, we used the software program Fityk (https://fityk.nieto.pl/) to deconvolve the broad ~7 Å peak into its separate kaolinite and chlorite components for each analysis. The mineralogical data arising from this method are referred to here as “Fityk data”. Unlike the method for the Highscore data, this technique does not provide relative abundances, but only confirms kaolinite presence.

Firstly, a pseudovoigt function was fitted to the ~7 Å peak using Fityk. Additional pseudovoigt functions were added until the residues between functions and data were of similar magnitude to those between the functions and background. A maximum of three pseudovoigt functions was identified, indicating possibly three distinct mineral phases. The d-spacing position of the maximum of each pseudovoigt function was recorded. Sample height displacement corrections, using the positions of quartz reflections as internal standards, were required due to variation in fossil topography and bedding plane angle.

The d-spacing positions of maxima of the pseudovoigt functions were partitioned into clusters using model-based clustering based on parameterized finite Gaussian mixture models in the R package ‘mclust’, v.5.4.2 (Scrucca et al., 2016), and the appropriate mineral was assigned to each (Kaolinite ~7.15 Å, Chlorite 7.08–7.14 Å; Moore and Reynolds, 1997). Prior to partitioning, outlying positions were removed, i.e., only pseudovoigt functions with maxima in the d-spacing range 7.05–7.19 Å were included (93% of functions). Models were estimated by
the EM algorithm initialized by hierarchical model-based agglomerative clustering. The optimal model was selected using the Bayesian Information Criterion (BIC). Defaults parameters were used for emControl, and no a priori subsets were specified. Three components were identified (log-likelihood=632.01, BIC=1229.88, Fig. S16); cluster one contained 155 observations (mean=7.09 Å, chlorite), cluster 2 contained 106 observations (mean=7.13 Å, chlorite), and cluster 3 contained 35 observations (mean=7.18 Å, kaolinite). Where two or three pseudovoigt functions were within one cluster for a single selected-area analysis, the position of the function with the larger area was chosen as their combined position.

Correspondence between Highscore and Fityk data

We investigated the correspondence between Highscore and Fityk data identifications of kaolinite (i.e., presence/absence). Categorization of presence/absence of kaolinite was similar in 66% of instances using Highscore and Fityk data. In the 33% of cases where the two methods disagreed, the Highscore data indicated kaolinite was present more often than not; i.e., 34 of 50 instances. Therefore, the Highscore method commonly misidentified chlorite as kaolinite, underscoring the robustness of our approach in testing relationships between mineralogy and fossil occurrences using two methods of mineral identification.

Addressing discrepancies between randomly oriented powder XRD and our in situ technique

Due to the orientation of clay minerals along the bedding plane, in situ selected-area XRD analyses may yield relative mineral abundances that do not correspond exactly to those obtained from randomly oriented powder analyses of matrix material. To examine any discrepancy between mineralogical abundances obtained from randomly-oriented powder XRD and our selected-area in situ method, XRD was performed on powders (ground to a grain size of approximately 10 μm and prepared as randomly oriented aggregates on single crystal silicon substrates 27 mm in diameter) created from matrix material surrounding two specimens of Marrella (USNM PAL 229990 and USNM PAL 230379). The results of these analyses were compared to those of the selected-area XRD analyses collected from three separate 7×1 mm areas of matrix surrounding each Marrella specimen (Table S1). The minerals identified in both powder and selected-area in situ analyses correspond closely in every case, with the exception of a systematic elevation in the absolute abundance of chlorite in the selected-area analyses of approximately 7–16%. We attribute this difference to preferred orientation effects.

1.3. Scanning Electron Microscopy-Energy Dispersive X-Ray Spectroscopy (SEM-EDS)

SEM-EDS analysis was undertaken on a Hitachi S3500-N scanning electron microscope (SEM) at the School of Earth Sciences, University of Bristol, UK and on an FEI 650 FEG-SEM at the Department of Earth Sciences, University of Oxford, UK. X-rays were detected and processed using a Thermo Fisher NSS EDS system at Bristol and an Oxford Instruments Aztec/X-Max 50 EDS system at Oxford. Samples were cleaned with a gas duster before shrouding in aluminum foil to assist with charge neutralization prior to insertion in the SEM. The SEM was operated in variable pressure mode to further neutralize charge build-up using a chamber pressure of 30 Pa of air (Bristol) and 50–70 Pa of water vapour (Oxford). Accelerating potential was 20 kV and beam current between 10–15 nA (Bristol) and ~5 nA (Oxford). Working Distance was 21 mm (Bristol) and 10 mm (Oxford). Individual frames were taken over an average of 20 full spectral X-ray images (and a backscatter electron image, Bristol) at 512×512 pixels and 100 s per image—a dwell time of 508 μs per pixel. The typical total run time for each specimen was 10–24
hours (Bristol) and 36–48 hours (Oxford) depending on the number of frames per specimen. All Images were montaged with a 5% overlap. Spectral processing—sum peak and escape peak removal and auto X-ray identification—was undertaken prior to image processing and subsequent conversion into RGB maps within the Bristol NSS system. Additionally, on the Oxford system background removal was performed using the Oxford Instruments TruMap algorithm.

1.4. Statistical Methodology
We used mixed effects logistic regression models to determine the nature of the relationship between selected-area type (i.e., fossil or matrix) and mineralogical composition. The identity of the rock specimen (n=15) from which fossil and matrix measurements derived was included as a random effect in the logistic model. We included this random effect because mineralogical measurements from the same rock sample were expected to pseudo-replicate each other due to shared diagenetic/metamorphic history.

We performed a suite of mixed effects logistic regression analyses with the relative abundance of minerals as fixed effects (Table S2). Relative abundances were subjected to arcsine transformation and included as predictors of selected-area type (i.e., fossil or matrix) in every combination, resulting in 128 possible models including one with no fixed effects. The predictors are compositional. To compensate, we also ran a suite of models with quartz removed (Table S4), which was shown not to be predictive of sample type (fossil or matrix) in the analyses that included all fixed effects. Quartz is an abundant mineral across all samples bar one. There were 64 possible models, including one with no fixed effects.

We also tested whether the presence of each mineral can distinguish fossils from their respective matrices. For these analyses, the relative abundance of each mineral from the Highscore data in each selected area (90 fossil and 57 matrix) was converted to a binary fixed effect (i.e., predictor) variable, indicating presence or absence of that mineral (Table S6). Only calcite, dolomite, kaolinite, and pyrite were considered because chlorite, muscovite, and quartz are present in nearly all samples. Models were run with all combinations of the four predictors, for a total of 16 models including one with no fixed effects. We also modelled the presence of kaolinite as the only predictor using Fityk data (Table S6).

Due to the singularity of the random effects, wherein estimated variance-covariance matrices had less than full rank, we implemented mixed effect logistic models using a partially Bayesian method that produces maximum a posteriori estimates using regularizing priors to force the random-effects variance-covariance matrices away from singularity. All models were implemented with functions in the ‘blme’ package (Chung et al., 2013) in the R programming language (R Core Team, 2020) using default priors.

Akaike’s Information Criterion (AIC) was estimated instead of corrected AIC, given the large number of measurements in the dataset, to determine the subset of models that received non-trivial weight (ΔAIC<10; for derivation and discussion of weights, see Burnham and Anderson, 2010). For fixed effects of models, we recorded coefficient estimates on the logit scale and 95% confidence interval bounds derived from bootstrapping for those models that received non-trivial weight. Models are listed in order of performance in Tables S3, S5, and S7.
2. Antibacterial properties of clays

Recent microbiological experiments have shown that the growth of the marine heterotrophic γ-proteobacterium *Pseudoalteromonas luteoviolacea*, known to decay marine animals today, is slowed in the presence of the clay minerals kaolinite and berthierine (McMahon et al., 2016). However, this is by no means the only study to evidence the antibacterial properties of clays. Kaolinite has also been shown to inhibit the growth of sulfate-reducing bacteria, autotrophic methanogens, and a heterotrophic soil bacterium (e.g., Wong et al., 2004; Wilson and Butterfield, 2014; Wu et al., 2014; Liu et al., 2016). The toxicity of the clays is primarily attributed to their metal cations (e.g., Wong et al., 2004; Morrison et al., 2016). Al\(^{3+}\) (kaolinite constituent) and Fe\(^{2+}\) (berthierine constituent) are known to be toxic to a diverse array of bacteria. In particular, excessive Fe\(^{2+}\) in aerobic conditions can cause oxidative damage to bacterial cells (Imlay et al., 1988; Guida et al., 1991; Kapoor and Arora, 1998; Amonette et al., 2003).

3. Other minerals with distinct fossil/matrix distributions

3.1. Apatite

Although no selected-area XRD analyses recorded apatite, SEM-EDS maps showed that phosphorus is present in the digestive systems of *Opabinia* (Fig. S8) and *Ottoia* (Fig. S10). This is consistent with previous reports of phosphate mineralization of digestive systems in *Opabinia* and other Burgess Shale fossils (e.g., Butterfield, 2002). Selective phosphatization of digestive systems is attributed to the lability of these tissues, and perhaps an internal source of phosphorus or unique internal gut microbiota (Butterfield, 2002).

3.2. Chlorite

Selected-area XRD data suggested that chlorite is statistically less abundant in fossils than in their respective matrices (Results, main paper). Evidence from BST deposits globally suggests matrices are enriched in the iron-rich clay berthierine (Anderson et al., 2018; Saleh et al., 2019). Berthierine forms as a product of kaolinite and Fe\(^{2+}\) in early diagenesis and transforms to the iron-rich chlorite chamosite in metamorphism (Bhattacharyya, 1983; Taylor, 1990; Taylor and Curtis, 1995; Fritz and Toth, 1997; Toth and Fritz, 1997; Rivard et al., 2013). Analysis of the relative intensities of the 002 (7.07 Å), 003 (4.72 Å), 004 (3.54Å), and 005 (2.83 Å) chlorite peaks can be used to determine its iron content (Brown and Brindley, 1980), \(y\) in the composition:

\[
(Mg,Al)_{6-2y}Fe_y(Si,Al)_{4}O_{10}(OH)_8.
\]

Our data suggested that chamosite forms a significant component of the chlorite in our samples: \(y\) can be up to 13 with a mean of 4 (stdev=3, n=145, Table S8). Kaolinite, known to be present in a proportion of our samples, has peaks which interfere with the 002 and 004 peaks of chlorite. However, the effect of any interference on our estimate of the chlorite iron content is insignificant. Removing samples with kaolinite (identified using the Fityk Data), resulted in a mean \(y\) of 4 (stdev=3, n=110). For this analysis, intensities corresponding to collection via a fixed divergence slit were used.
Bonding of kaolinite to fossil organic matter early in diagenesis may have prevented not only transformation of fossil-associated kaolinite to illite/muscovite in metamorphism (Discussion, main paper) but also transformation to berthierine in early diagenesis. Emerging from early diagenesis, therefore, matrices may have been enriched in berthierine compared to fossils (which were enriched in kaolinite). Thus, metamorphic transformation of berthierine to chamosite may account for the higher chlorite abundances which distinguish matrices from fossils in our data. Iron content within chlorite, however, does not vary substantially between fossils and matrices (Fig. S17), suggesting transformations during metamorphism of kaolinite to lower iron content chlorite variants (Boles and Franks, 1979; Ehrenberg et al., 1993) were also inhibited by kaolinite bonding with fossil organic matter.

If the same logic were applied to muscovite distributions, we might expect muscovite to be statistically higher in abundance in matrices versus fossils as well—a pattern not supported by our data. However, detrital, diagenetic, and metamorphic minerals all contribute to what ultimately becomes muscovite. Thus, it is difficult to attribute modern distributions of this mineral to specific transformational pathways. Masking-effects from other mineralogical transformations probably render any contribution from kaolinite difficult to observe, especially given the precision of our analyses.

### 3.3. Dolomite

Selected-area XRD data suggested that dolomite is statistically both more commonly present and more abundant in fossils than in their respective matrices (Results, main paper). The formation of dolomite could have occurred either in early diagenesis or in late diagenesis/metamorphism. The latter possibility would require conversion of a pre-existing carbonate mineral (i.e., calcite or aragonite) to dolomite, meaning a carbonate at least was precipitated during early diagenesis. Selected-area XRD data suggested calcite does not distinguish between fossils and matrices (Results, main paper), possibly arguing against preferential conversion of calcite in one or other setting (i.e., fossils or matrices).

An early diagenetic origin for dolomite (or CaCO$_3$) may relate to geochemical changes triggered upon degradation of organic matter. Evaporite fluid inclusion data indicate that early/mid-Cambrian seawater was relatively poor in sulfate (Brennan et al., 2004). Thus, microbial degradation of an organic matter-rich region of the sediment (such as a decaying carcass) may have depleted sulfate through sulfate reduction and led to methanogenesis (at least locally). As a consequence, the anaerobic oxidation of methane may have featured more commonly as soft tissues decomposed in lower-sulfate seas. This process is known to release significant amounts of alkalinity and dissolved inorganic carbon, and to result in the precipitation of CaCO$_3$ and some so-called “organogenic” dolomite (Compton, 1988; Knittel & Boetius, 2009).

### 3.4. Pyrite

Selected-area XRD data suggested that pyrite is statistically both more commonly present and more abundant in fossils than in their respective matrices (Results, main paper), supporting a role previously identified for pyritization of fossil tissues (e.g., Briggs, 2003; Garcia-Bellido and Collins, 2006). However, individual pyrite occurrences are comparatively rare. Of the 147 selected-area analyses, only 27 recorded pyrite (18.1%). Of these, all were associated with fossil
selected-areas apart from three (Table S1). Sample sizes were insufficient to assess statistically whether particular taxa are more prone to pyritization than others, although qualitatively pyrite does seem more commonly present in *Opabinia* (specifically USNM PAL 155600).

In addition, SEM-EDS data qualitatively showed that pyrite may be restricted to particular anatomical features. Specifically, Figs. S7 and S8 show enrichments of iron in the eyes of *Opabinia*. Pyrite was identified in selected-area XRD covering these anatomical features (Table S1, USNM PAL 139217 selected-area “body 1”, USNM PAL 155600 selected areas “eyes_12mm” and “eyesnew_7mm”). In this case the visual pigment melanin (Glass et al., 2012) may have provided an organic substrate for pyritization. SEM-EDS data also pointed to iron enrichments in digestive systems of *Canadia* (Fig. S1) *Marrella* (Fig. S4), *Opabinia* (Fig. S8), and *Ottoia* (Fig. S11, S12). In other cases, however, patterns of pyritization (as reflected by iron enrichments) do not necessarily follow morphology (e.g., Fig. S15).

4. Summaries of mineralogy by taxon

All XRD data presented in these summaries derive from the Highscore data (Table S1). The silhouettes in Fig. 2 were obtained from burgess-shale.rom.on.ca.

4.1. Canadia

The selected areas of all three specimens and their matrices are dominated by muscovite (43–80%), quartz (16–44%), and chlorite (0–28%). Muscovite abundances are systematically lower in USNM PAL 199758 and its matrix than in the others (muscovite USNM PAL 199758 mean=48.7, stdev=7.2 n=9, versus others mean=58.8, stdev=9.3, n=21), whereas chlorite and quartz are elevated (chlorite USNM PAL 199758 mean=17.4, stdev=6.5, n=9, versus others mean=11.6, stdev=6.0, n=21; quartz USNM PAL 199758 mean=30.9, stdev=5.4, n=9, versus others mean=26.3, stdev=8.1, n=21). Neither calcite nor dolomite exceed 3% in any fossil or matrix analysis: Calcite is present across 77% of all selected areas but dolomite is only present in those of USNM PAL 199758 that covered the bristles. Pyrite is present occasionally, but only in fossils and always in quantities ≤1%. SEM-EDS data showed iron can be enriched in the digestive system (central axis and adjacent areas; Fig. S1). Kaolinite, which occurs in abundances ≤13% was found primarily in selected areas encompassing the digestive system, although it is present in all anatomical features in USNM PAL 199758. Kaolinite was also recorded in one matrix selected area from USNM PAL 198724. SEM-EDS showed elevated concentrations of aluminum in the vicinity of the digestive system consistent with the mineralogical observations (Figs. S1–S3).

4.2. Marrella

Selected areas of all specimens of *Marrella* and their surrounding matrices are dominated by muscovite (19–83%). Chlorite (4–36%) and quartz (10–55%, but absent in one selected-area of USNM PAL 166587) are also common. Muscovite (63–68%) and quartz (18–25%) abundances show less variability in USNM PAL 230379. Both calcite and dolomite are confined to USNM PAL 166587 and USNM PAL 229990 (≤4%), but absent in USNM PAL 230379, although they were observed in XRD analyses of matrix powders from that specimen. Pyrite was only recorded in USNM PAL 166587 where it is present in selected areas encompassing one side of the central axis and the head region, always in an abundance of 3%. SEM-EDS data also indicated
areas that contain kaolinite cover enrichments of iron through this specimen (Fig. S4) indicative of pyritization. Kaolinite is present in USNM PAL 229990 and USNM PAL 230379 in abundances ≤4% and is normally confined to the digestive system (stomach, cephalic canals, and remainder of the gut trace). Trace amounts (<1% abundance) of kaolinite were also recorded by XRD in the lower body of USNM PAL 229990. Kaolinite is present in USNM PAL 166587 again in selected-areas encompassing its digestive system (11–12%). Consistent with these mineralogical observations, SEM-EDS showed elevated aluminum in the digestive systems of all specimens (Figs. S4–S6).

4.3. *Opabinia*

The two specimens and their respective matrices are dominated by muscovite (39–79%), chlorite (0–30%) and quartz (12–44%). Muscovite is elevated in USNM PAL 139217 (mean=65.8, stdev=10.6, n=11) compared to USNM PAL 155600 (mean=50.1, stdev=10.0, n=16), whereas chlorite is lower in abundance (USNM PAL 139217 mean=8.8, stdev=3.7, n=11, versus USNM PAL 155600 mean=21.6, stdev=6.1, n=16). Calcite is present in all selected areas of USNM PAL 155600 (<2%) with dolomite in 81% of selected-areas (≤1%), but both are absent in USNM PAL 139217. Pyrite is present in 85% of selected areas of USNM PAL 155600 (≤2%) and is also present in a selected area of its matrix and a selected area covering the eyes of USNM PAL 139217. SEM-EDS showed corresponding enrichments of iron along the gut traces and prominently in the eyes of both specimens (Figs. S7, S8). Kaolinite is fairly common but is only present on fossils (50% of fossil selected areas on USNM PAL 139217 and 54% on USNM PAL 155600). SEM-EDS showed aluminum to be present within the gut traces of both specimens (Figs. S7, S8).

4.4. *Ottoia*

Muscovite (27–74%), chlorite (4–37%), and quartz (15–28%) are the most abundant minerals in the four specimens. Muscovite is elevated in USNM PAL 188616 (mean=62.3, stdev=3.2, n=8) and USNM PAL 198565 (mean=66.2, stdev=5.6, n=6) compared to the others (USNM PAL 188617 mean=49.0, stdev=12.2, n=8; USNM PAL 198577 mean=50.0, stdev=11.6, n=10). The lowest chlorite content was recorded by XRD in selected areas of USNM PAL 198565 (mean=8.8, stdev=5.2, n=6) and the highest across those of USNM PAL 188617 (mean=24.8, stdev=9.0, n=8); those of the other two specimens yielded intermediate values (USNM PAL 188616 mean=13.0, stdev=2.7, n=8; USNM PAL 198577 mean=14.8, stdev=6.7, n=10). Quartz is slightly elevated in USNM PAL 198577 (mean=29.9, stdev=14.0, n=10) compared to the other specimens (USNM PAL 188616 mean=22.6, stdev=3.0, n=8; USNM PAL 188617 mean=21.375, stdev=4.8, n=8; USNM PAL 198565 mean=21.7, stdev=3.0, n=6). Calcite is a minor constituent of all specimens, reaching a maximum in USNM PAL 188617 (commonly 3–4%); SEM-EDS maps of calcium revealed a striking contrast between fossil and matrix for this specimen (Fig. S10) and also USNM PAL 198577 (Fig. S12). SEM-EDS data also showed the extremities of USNM PAL 198565 are defined by enrichments of calcium (Fig. S11). Dolomite is relatively common (≤1%) although it is absent from USNM PAL 198565. Pyrite is only present in USNM PAL 188617, where XRD recorded it in both fossil and matrix. However, SEM-EDS data suggested it is also present in the digestive systems of USNM PAL 198565 and USNM PAL 198577 (Figs. S11, S12), contrasting spatially in USNM PAL 198577 with enrichments of carbon, but coinciding with concentrations of aluminum in both specimens. Kaolinite is present in abundances ≤10% in all specimens but only in fossils: 83% of selected areas that contain kaolinite cover digestive systems. Aluminum is abundant in the gut trace of all
specimens (Figs. S9–S12). Finally, SEM-EDS data suggested enrichments of phosphorus likely representing apatite in the digestive system of USNM PAL 198617 (Fig. S10).

4.5. *Pikaia*

The minerals muscovite (33–69%), chlorite (7–37%), and quartz (12–30%) are dominant. Muscovite and chlorite abundances vary inversely: The highest abundances of muscovite (mean=57.9, stdev=5.6, n=15) and lowest chlorite (mean=14.3, stdev=6.9, n=15) are present in USNM PAL 198688, whereas USNM PAL 202220 has the lowest muscovite (mean=45.0, stdev=7.9, n=8) and highest chlorite (mean=27.1, stdev=6.8, n=8). The abundances in USNM PAL 198692 are intermediate (muscovite mean=49.3, stdev=10.3, n=8; chlorite mean=19.0, stdev=5.1, n=7). Minor calcite is almost ubiquitous (≤4%), absent only in one matrix selected area of USNM PAL 198688. SEM-EDS maps showed calcium contrasts between fossils and matrices (Figs. S13–S15; also observed by Conway Morris and Caron, 2012). Dolomite, in contrast, is rare and was only recorded by XRD in USNM PAL 202220 (≤1%), where it was observed in all analyses covering the fossil but in only one matrix analysis. Pyrite is only present in two selected areas of the fossil in USNM PAL 198688 (≤4%). SEM-EDS recorded enrichments of iron in this specimen (Fig. S13). Iron also defines a linear feature at the posterior end of USNM PAL 198692 (Fig. S14), which may correspond to the nerve chord and/or notochord. Kaolinite was recorded by XRD in all specimens and reaches relatively high abundances (≤28%). It is present in selected areas covering the fossils, except in USNM PAL 202220 where it is also present in 66.7% of matrix analyses. SEM-EDS suggested USNM PAL 198688 had one area of particular aluminum enrichment (Fig. S13). SEM-EDS also detected minor phosphorus (apatite?) enrichment traversing the trunk of USNM PAL 202220 (Fig. S15).

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Table S1. Mineralogical composition from selected-area X-ray diffraction. Abbreviations: Irr = irradiated, Pt = part, Cpt = counterpart, Cal = calcite, Chl = chlorite, Dol = dolomite, Kaol = kaolinite, Musc = muscovite, Pyr = pyrite, Qtz = quartz, Tot = total, Clust = cluster.

| Fossil Details | Highscore Data | Fityk Data |
|----------------|----------------|-------------|
| Fossil | Selected Area | Irr Width | Fig S1-S15 Location | Pt/ Cpt | Fossil/ Matrix | Digestive System | Cal % | Chl % | Dol % | Kaol % | Musc % | Pyr % | Qtz % | Tot | Clust 1 Chl 7.09 | Clust 2 Chl 7.13 | Clust 3 Kaol 7.17 |
| Canadia | matrix1 | 7 | m | | | | 3 | 9 | 0 | 0 | 54 | 0 | 34 | 100 | 7.091 | 7.138 |
| USNM | matrix2 | 7 | m | | | | 1 | 15 | 0 | 0 | 67 | 0 | 17 | 100 | 7.094 | 7.135 |
| PAL | matrix3 | 7 | m | | | | 2 | 17 | 0 | 0 | 55 | 0 | 26 | 100 | 7.105 | | |
| 198723 | body1 | 7 | 1 | r | d | 0.5 | 10 | 0 | 8 | 58 | 0 | 24 | 100.5 | 7.085 | 7.162 |
| body2 | 7 | 2 | r | | | | 2 | 15 | 0 | 0 | 60 | 0.5 | 24 | 101.5 | 7.100 | 7.177 |
| body3 | 7 | 3 | r | d | 0 | 8 | 0 | 0 | 70 | 0 | 21 | 99 | 7.108 | 7.185 |
| body4 | 7 | 4 | r | d | 1 | 8 | 0 | 0 | 64 | 0 | 26 | 99 | 7.068 | | |
| body5 | 7 | 5 | r | d | 1 | 15 | 0 | 0 | 50 | 0.5 | 33 | 99.5 | | | |
| body6 | 7 | 6 | r | | 3 | 13 | 0 | 0 | 50 | 0 | 34 | 100 | | | |
| Canadia | matrix1 | 7 | a | m | | | 0 | 11 | 0 | 0 | 71 | 0 | 18 | 100 | 7.107 | 7.153 |
| USNM | matrix2 | 7 | a | m | | | 2 | 17 | 0 | 0 | 65 | 0 | 16 | 100 | 7.076 | 7.123 |
| PAL | matrix3 | 7 | a | m | | | 2 | 14 | 0 | 12 | 37 | 0 | 35 | 100 | | | |
| 198724 | matrix4 | 7 | a | m | | | 0 | 10 | 0 | 0 | 64 | 0 | 27 | 101 | 7.136 | | |
| matrix5 | 7 | d | m | | 0 | 0 | 0 | 0 | 80 | 0 | 16 | 100 | 7.102 | 7.140 |
| matrix6 | 7 | d | m | | 2 | 26 | 0 | 0 | 55 | 0 | 17 | 100 | 7.097 | 7.136 |
| matrix7 | 7 | d | m | | 0 | 17 | 0 | 0 | 62 | 0 | 21 | 100 | 7.084 | 7.114 | 7.158 |
| body1 | 7 | 1 | a | r | 0 | 9 | 0 | 7 | 50 | 0 | 34 | 100 | 7.075 | 7.169 |
| body2 | 7 | 2 | a | r | 2 | 13 | 0 | 13 | 51 | 1 | 20 | 100 | 7.078 | 7.166 |
| body3 | 7 | 3 | a | r | 3 | 0 | 0 | 0 | 59 | 0 | 38 | 100 | | | |
| body4 | 7 | 4 | d | r | 0 | 0 | 0 | 0 | 56 | 0 | 44 | 100 | | | |
| body5 | 7 | 5 | d | r | 2 | 13 | 0 | 0 | 57 | 0 | 28 | 100 | 7.076 | | |
| Canadia | matrix | 7 | m | | | | 2 | 27 | 0 | 0 | 43 | 0 | 27 | 99 | 7.070 | 7.148 |
| USNM | matrix2 | 7 | m | | | | 3 | 28 | 0 | 0 | 43 | 0 | 26 | 100 | 7.091 | 7.128 | 7.182 |
| PAL | matrix3 | 7 | m | | | | 0.5 | 13 | 0 | 0 | 48 | 0.5 | 38 | 100 | 7.082 | 7.118 |
| 199758 | edgeofbristles | 7 | 1 | m | | | 1 | 21 | 0 | 0 | 46 | 0 | 32 | 100 | 7.096 | 7.170 |
| centre | 7 | 2 | r | | 1 | 14 | 0 | 0 | 63 | 0 | 22 | 100 | 7.112 | 7.173 |
| bristlesright | 7 | 3 | r | | 1 | 13 | 0.5 | 0.5 | 58 | 0 | 28 | 101 | 7.083 | 7.133 | 7.177 |
| bristlesright 2 | 7 | 4 | r | | 3 | 18 | 0.5 | 2 | 43 | 1 | 34 | 101.5 | 7.079 | 7.115 |
| centre2 | 7 | 5 | r | d | 2 | 12 | 0.5 | 2 | 45 | 0.5 | 37 | 99 | 7.088 | 7.171 |
| edgeofbristles 2 | 12 | 6 | r | | 2 | 11 | 0 | 4 | 49 | 0 | 34 | 100 | 7.083 | 7.175 |
| Marrella | matrix1 | 7 | a | m | | | 0 | 21 | 0 | 0 | 52 | 0 | 27 | 100 | | | |
| USNM | matrix2 | 7 | d | m | | | 0 | 26 | 0 | 0 | 56 | 0 | 18 | 100 | 7.091 | | |
| PAL | matrix3 | 7 | d | m | | | 1 | 24 | 0 | 0 | 54 | 0 | 21 | 100 | 7.085 | 7.127 |
| 166587 | matrix4 | 7 | d | m | | | 3 | 0 | 0 | 0 | 65 | 0 | 24 | 100 | 7.083 | 7.140 |
| matrix5 | 7 | a | m | | | | 0 | 8 | 0 | 0 | 44 | 0 | 48 | 100 | 7.069 | 7.120 |
| Fossil      | Selected Area | Irr Width | Fig S1-S15 Location | Pt/ Cpt | Fossil/ Matrix | Digestive System | Cal % | Chl % | Dol % | Kaol % | Musc % | Pyr % | Qtz % | Tot | Clust 1 Chl 7.09 | Clust 2 Chl 7.13 | Clust 3 Kaol 7.17 |
|------------|---------------|-----------|---------------------|--------|---------------|------------------|-------|-------|-------|--------|--------|-------|-------|-----|-----------------|-----------------|-----------------|
| matrix6    |              | 7         | a                   | m      |               |                  | 0     | 7     | 0     | 0      | 83     | 0     | 10    | 100 | 7.141           |                 |                 |
| body1      |              | 7         | 1                   | a      | f             | d                | 0     | 13    | 0     | 11     | 46     | 0     | 30    | 100 | 7.084           |                 |                 |
| body2      |              | 7         | 2                   | a      |                | r                | 0     | 15    | 0     | 12     | 34     | 0     | 39    | 100 | 7.070           |                 |                 |
| body3      |              | 7         | 3                   | a      |                | r                | 2     | 18    | 4     | 38     | 0      | 37    | 99    | 7.101 |                 |                 |                 |
| body4      |              | 7         | 4                   | a      |                | r                | 0     | 17    | 0     | 0      | 40     | 3     | 40    | 100 | 7.180           |                 |                 |
| body5      |              | 7         | 5                   | d      |                | r                | 0     | 15    | 0     | 0      | 35     | 0     | 50    | 100 | 7.139           |                 |                 |
| body6      |              | 7         | 6                   | d      |                | r                | 0     | 14    | 0     | 12     | 19     | 0     | 55    | 100 | 7.130           |                 |                 |
| body7      |              | 7         | 7                   | d      |                | r                | 0     | 36    | 0     | 0      | 64     | 0     | 100   |     | 7.171           |                 |                 |
| body8      |              | 7         | 8                   | d      |                | r                | 1     | 24    | 0     | 0      | 54     | 3     | 18    | 100 | 7.086           |                 |                 |
| body9      |              | 7         | 9                   | d      |                | r                | 0     | 9     | 0     | 0      | 66     | 0     | 25    | 100 | 7.094           |                 |                 |
| Marrella   | powder       |           |                     | m      |               |                  | 3     | 4     | 2     | 0      | 39     | 0     | 53    | 101 | 7.066           |                 |                 |
| Marrella   | powder       |           |                     | m      |               |                  | 4     | 8     | 1     | 0      | 63     | 0     | 25    | 101 | 7.066           |                 |                 |
| USNM       | matrix1      | 7         |                     | m      |               |                  | 0.5   | 18    | 1     | 0      | 37     | 0     | 44    | 100.5 | 7.089       | 7.125           |                 |
| PAL        | matrix2      | 7         |                     | m      |               |                  | 0.5   | 18    | 1     | 0      | 63     | 0     | 17    | 99.5  | 7.098       | 7.139           |                 |
| 229990     | matrix3      | 7         |                     | m      |               |                  | 1     | 20    | 1     | 0      | 58     | 0     | 20    | 100  | 7.097       | 7.130           |                 |
| head_scan1 |                     | 7         | 1                   | r      |                | d                | 0     | 11    | 0.5   | 4      | 56     | 0     | 29    | 100.5 | 7.080       |                 | 7.171           |
| body_scan_center_1 |   | 7         | 2                   | r      |                | d                | 1     | 12    | 1     | 2      | 60     | 0     | 25    | 101  | 7.097       | 7.151           |                 |
| body_scan_right_1 |   | 7         | 3                   | r      |                |                  | 1     | 15    | 1     | 0.5    | 62     | 0     | 22    | 101.5 | 7.098      | 7.151           |                 |
| Marrella   | powder       |           |                     | m      |               |                  | 4     | 8     | 1     | 0      | 63     | 0     | 25    | 101  | 7.066           |                 |                 |
| USNM       | matrix1      | 7         |                     | m      |               |                  | 0.5   | 18    | 1     | 0      | 37     | 0     | 44    | 100.5 | 7.089       | 7.125           |                 |
| PAL        | matrix2      | 7         |                     | m      |               |                  | 0.5   | 18    | 1     | 0      | 63     | 0     | 17    | 99.5  | 7.098       | 7.139           |                 |
| 230379     | matrix3      | 7         |                     | m      |               |                  | 1     | 20    | 1     | 0      | 58     | 0     | 20    | 100  | 7.097       | 7.130           |                 |
| head_scan1 |                     | 7         | 1                   | r      |                | d                | 0     | 12    | 0     | 0      | 68     | 0     | 19    | 99    | 7.092       | 7.140           |                 |
| head_scan_2 |                     | 7         | 2                   | r      |                |                  | 0     | 15    | 0     | 0      | 65     | 0     | 21    | 101  | 7.113       |                 | 7.158           |
| upper-body_scan_1 |   | 7         | 3                   | r      |                | d                | 0     | 15    | 0     | 0.5    | 66     | 0     | 18    | 99.5  | 7.089       | 7.141           |                 |
| lower-body_scan_1 |   | 7         | 4                   | r      |                |                  | 0     | 10    | 0     | 0      | 66     | 0     | 24    | 100  | 7.070       | 7.116           |                 |
| Opabinia   | matrix1      | 7         |                     | m      |               |                  | 0     | 9     | 0     | 0      | 78     | 0     | 12    | 99    | 7.088       | 7.130           |                 |
| USNM       | matrix2      | 7         |                     | m      |               |                  | 0     | 8     | 0     | 0      | 48     | 0     | 44    | 100  | 7.071       | 7.126           |                 |
| PAL        | matrix3      | 7         |                     | m      |               |                  | 0     | 8     | 0     | 0      | 79     | 0     | 13    | 100  | 7.090       | 7.128           |                 |
| 139217     | body1        | 7         | 1                   | r      |                |                  | 0     | 13    | 0     | 18     | 50     | 2     | 17    | 100  | 7.092       |                 | 7.154           |
| body2      |              | 7         | 2                   | r      |                |                  | 0     | 9     | 0     | 5      | 65     | 0     | 21    | 100  | 7.089       | 7.125           |                 |
| body3      |              | 7         | 3                   | r      |                | d                | 0     | 0     | 0     | 5      | 70     | 0     | 25    | 100  | 7.099       |                 | 7.171           |
| body4      |              | 7         | 4                   | r      |                | d                | 0     | 11    | 0     | 0      | 71     | 0     | 18    | 100  | 7.090       | 7.138           |                 |
| body5.12mm |              | 12        | 5                   | r      |                | d                | 0     | 10    | 0     | 0      | 77     | 0     | 14    | 101  | 7.093       | 7.148           |                 |
| body6.12mm |              | 12        | 6                   | r      |                | d                | 0     | 5     | 0     | 0      | 61     | 0     | 34    | 100  | 7.104       | 7.152           |                 |
| body7.22m  |              | 22        | 7                   | r      |                | d                | 0     | 13    | 0     | 0      | 59     | 0     | 28    | 100  | 7.075       | 7.150           |                 |
| Fossil   | Selected Area | IRR Width | Fig S1-S15 Location | Pt/ Cpt | Fossil/ Matrix | Digestive System | Cal % | Chl % | Dol % | Kaol % | Musc % | Pyr % | Qtz % | Tot | Clust 1 Chl | Clust 2 Chl | Clust 3 Kaol |
|----------|---------------|-----------|---------------------|--------|----------------|------------------|------|------|------|-------|-------|------|------|-----|-------------|-------------|--------------|
| Opabinia | matrix        | 7         | m                   | 1      | 20             | 0                | 66   | 0    | 17   | 100   | 7.088 | 7.127 | USNM |              |              |              |
| USNM     | matrix2       | 7         | m                   | 2      | 28             | 1                | 0    | 39   | 0    | 100   | 7.089 | 7.126 | PAL   |              |              |              |
| Ottoia   | eyes_12mm     | 12        | 1                   | 1      | 16             | 0.5              | 57   | 1    | 25   | 100   | 7.106 | 7.147 | 155600 |              |              |              |
| Ottoia   | eyesnew_7mm   | 7         | 2                   | 1      | 17             | 1                | 3    | 43   | 2    | 100   | 7.100 | 7.189 | USNM |              |              |              |
| Ottoia   | gut_22mm      | 22        | 3                   | 1      | 23             | 0.5              | 58   | 0    | 5     | 24    | 100   | 7.083 | 7.153 | USNM |              |              |              |
| Ottoia   | flapnew_2_7mm | 7         | 4                   | 1      | 23             | 1                | 3    | 43   | 1    | 100   | 7.090 | 7.141 | PAL   |              |              |              |
| Ottoia   | flapnew3_7mm  | 7         | 4                   | 1      | 23             | 0.5              | 5     | 2    | 54   | 100   | 7.090 | 7.143 | USNM |              |              |              |
| Ottoia   | flapnew 7mm   | 7         | 5                   | 1      | 11             | 0                | 5    | 43   | 0    | 100   | 7.088 | 7.128 | 188616 |              |              |              |
| Ottoia   | partialgut    | 7         | 6                   | 1      | 27             | 0.5              | 50   | 1    | 21   | 100   | 7.111 | 7.158 | USNM |              |              |              |
| Ottoia   | flap_22mm     | 22        | 7                   | 1      | 27             | 0.5              | 43   | 2    | 26   | 100   | 7.086 | 7.120 | PAL   |              |              |              |
| Ottoia   | gut22         | 22        | 8                   | 1      | 27             | 0.5              | 43   | 2    | 26   | 100   | 7.086 | 7.120 | USNM |              |              |              |
| Ottoia   | gut12mm       | 12        | 10                  | 1      | 21             | 1                | 4    | 3    | 3    | 100   | 7.085 | 7.139 | PAL   |              |              |              |
| Ottoia   | gut3_22mm     | 22        | 11                  | 1      | 15             | 0                | 62   | 1    | 21   | 100   | 7.090 | 7.128 | USNM |              |              |              |
| Ottoia   | gutnew2_7mm   | 7         | 12                  | 1      | 26             | 1                | 3    | 44   | 0    | 23    | 99    | 7.100 | 7.169 | USNM |              |              |              |
| Ottoia   | gut2         | 7         | m                   | 2      | 19             | 0.5              | 58   | 0    | 21   | 100   | 7.098 | 7.123 | USNM |              |              |              |
| Ottoia   | gut3_7mm      | 7         | m                   | 2      | 19             | 0.5              | 43   | 2    | 26   | 100   | 7.089 | 7.124 | PAL   |              |              |              |
| Ottoia   | gut3_7mm      | 7         | m                   | 2      | 19             | 0.5              | 58   | 0    | 21   | 100   | 7.090 | 7.124 | USNM |              |              |              |
| Ottoia   | body2_7mm     | 7         | 4                   | 1      | 26             | 1                | 3    | 44   | 0    | 23    | 99    | 7.100 | 7.087 | USNM |              |              |              |
| Ottoia   | matrix        | 7         | m                   | 2      | 19             | 0.5              | 56   | 0    | 21   | 100   | 7.090 | 7.128 | PAL   |              |              |              |
| Ottoia   | matrix2       | 7         | m                   | 2      | 19             | 0.5              | 58   | 0    | 21   | 100   | 7.090 | 7.128 | USNM |              |              |              |
| Ottoia   | matrix3       | 7         | m                   | 2      | 19             | 0.5              | 58   | 0    | 21   | 100   | 7.090 | 7.128 | PAL   |              |              |              |
| Ottoia   | body3_7mm     | 7         | m                   | 2      | 19             | 0.5              | 58   | 0    | 21   | 100   | 7.090 | 7.128 | USNM |              |              |              |
| Fossil Details | Highscore Data | Fityk Data |
|---------------|---------------|------------|
| Fossil | Selected Area | Irr Width | Fig S1-S15 Location | Pt/ Cpt | Fossil/ Matrix | Digestive System | Cal % | Chl % | Dol % | Kaol % | Musc % | Pyr % | Qtz % | Tot | Clust 1 Chl 7.09 | Clust 2 Chl 7.13 | Clust 3 Kaol 7.17 |
| PAL | matrix3 | 7 | m | 3 | 6 | 0 | 0 | 69 | 0 | 22 | 100 | 7.071 | 7.113 | 7.179 |
| 198565 | backbody1 | 7 | 1 | f | 1 | 8 | 0 | 7 | 64 | 0 | 19 | 99 | 7.103 | 7.162 |
| gut1 | 7 | 2 | f | d | 0 | 4 | 0 | 6 | 66 | 0 | 24 | 100 | 7.123 | 7.181 |
| backbody2 | 7 | 3 | f | 1 | 8 | 0 | 0 | 67 | 0 | 24 | 100 | 7.099 | 7.137 | 7.174 |
| Ottoia | matrix1 | 7 | m | 3 | 23 | 1 | 0 | 56 | 0 | 16 | 99 | 7.087 | 7.132 |
| USNM | matrix2 | 7 | m | 3 | 14 | 0 | 0 | 59 | 0 | 22 | 98 | 7.082 | 7.129 |
| PAL | matrix3 | 7 | m | 0 | 24 | 0 | 0 | 22 | 0 | 54 | 100 | 7.096 | 7.133 |
| 198577 | body1 | 7 | 1 | f | 2 | 9 | 0 | 0 | 40 | 0 | 50 | 101 | 7.100 | 7.119 |
| body2 | 7 | 2 | f | d | 2 | 15 | 1 | 4 | 55 | 0 | 22 | 99 | 7.080 | 7.123 |
| body3 | 7 | 3 | f | d | 1 | 4 | 0 | 0 | 49 | 0 | 45 | 99 | 7.084 | 7.128 |
| body4 | 7 | 4 | f | d | 0 | 7 | 0 | 4 | 63 | 0 | 26 | 100 | 7.079 | 7.123 |
| body5 | 7 | 5 | f | d | 3 | 14 | 1 | 5 | 54 | 0 | 23 | 100 | 7.087 | 7.132 |
| body6 | 7 | 6 | f | d | 2 | 19 | 0 | 5 | 52 | 0 | 22 | 100 | 7.096 | 7.140 |
| body7 | 7 | 7 | f | 3 | 19 | 0 | 9 | 50 | 0 | 19 | 100 | 7.084 | 7.123 |
| Pikaia | matrix1 | 7 | a | m | 1 | 24 | 0 | 0 | 56 | 0 | 19 | 100 | 7.090 | 7.117 | 7.179 |
| USNM | matrix2 | 7 | a | m | 1 | 16 | 0 | 0 | 55 | 0 | 28 | 100 | 7.070 | 7.149 |
| PAL | matrix3 | 7 | a | m | 2 | 10 | 0 | 0 | 68 | 0 | 21 | 101 | 7.089 | 7.120 |
| 198688 | matrix4 | 7 | d | m | 0 | 7 | 0 | 0 | 63 | 0 | 30 | 100 | 7.100 | 7.141 |
| matrix5 | 7 | d | m | 3 | 21 | 0 | 0 | 58 | 0 | 18 | 100 | 7.115 | 7.160 |
| matrix6 | 7 | d | m | 2 | 23 | 0 | 0 | 56 | 0 | 19 | 100 | 7.090 | 7.148 |
| body1 | 7 | 1 | a | f | 3 | 10 | 0 | 0 | 58 | 0 | 29 | 100 | 7.090 | 7.147 |
| body2 | 7 | 2 | a | f | 2 | 9 | 0 | 0 | 64 | 1 | 24 | 100 | 7.090 | 7.147 |
| body3 | 7 | 3 | a | f | 2 | 11 | 0 | 4 | 56 | 0 | 27 | 100 | 7.090 | 7.147 |
| body4 | 7 | 4 | a | f | 2 | 7 | 0 | 13 | 56 | 0 | 22 | 100 | 7.097 | 7.139 |
| body5 | 7 | 5 | d | f | 2 | 13 | 0 | 11 | 52 | 0 | 23 | 101 | 7.088 | 7.112 |
| body6 | 7 | 6 | d | f | 2 | 29 | 0 | 0 | 55 | 0 | 14 | 100 | 7.089 | 7.113 | 7.159 |
| body7 | 7 | 7 | d | f | 1 | 13 | 0 | 19 | 50 | 0 | 4 | 12 | 99 | 7.085 | 7.128 |
| body8 | 7 | 8 | d | f | 2 | 7 | 0 | 0 | 69 | 0 | 22 | 100 | 7.086 | 7.136 |
| body9 | 7 | 9 | d | f | 1 | 14 | 0 | 6 | 53 | 0 | 26 | 100 | 7.080 | 7.171 |
| Pikaia | matrix1 | 7 | m | 1 | 18 | 0 | 0 | 60 | 0 | 20 | 99 | 7.090 | 7.144 |
| USNM | matrix2 | 7 | m | 2 | 18 | 0 | 0 | 57 | 0 | 23 | 100 | 7.090 | 7.121 |
| PAL | matrix3 | 7 | m | 2 | 22 | 0 | 0 | 55 | 0 | 21 | 100 | 7.080 | 7.155 |
| 198602 | body1 | 7 | 1 | f | 4 | 20 | 0 | 28 | 33 | 0 | 15 | 100 | 7.070 | 7.112 |
| body2 | 7 | 2 | f | 3 | 27 | 0 | 12 | 39 | 0 | 20 | 101 | 7.060 | 7.127 |
| body3 | 7 | 3 | f | 4 | 18 | 0 | 17 | 45 | 0 | 16 | 100 | 7.088 | 7.120 |
| Fossil       | Selected Area | Area | Width | Location | Pt/ Cpt | Fossil/ Matrix | Digestive System | Cal % | Chl % | Dol % | Kaol % | Musc % | Pyr % | Qtz % | Tot % | Clust 1 Chl | Clust 2 Chl | Clust 3 Kaol |
|-------------|---------------|------|-------|----------|--------|----------------|-------------------|-------|-------|-------|--------|--------|-------|-------|-------|-------------|-------------|--------------|
| body4       |               | 7    | 4     | f        |         |                |                   | 4     | 10    | 0     | 5      | 56     | 0     | 25    | 100   | 7.110       | 7.139       |              |
| Pikaia matrix |             | 7    | m     |          |        |                |                   | 3     | 36    | 0.5   | 0      | 39     | 0     | 22    | 100.5 | 7.077       | 7.115       |              |
| USNM matrix3 |             | 7    | m     |          |        |                |                   | 2     | 23    | 0     | 5      | 52     | 0     | 17    | 99    | 7.110       |              |              |
| PAL matrix4 |             | 7    | m     |          |        |                |                   | 4     | 22    | 0     | 2      | 46     | 0     | 26    | 100   | 7.060       | 7.180       |              |
| 202220      | myomeres     | 7    | 1     | f        |         |                |                   | 2     | 24    | 1     | 4      | 50     | 0     | 19    | 100   | 7.070       | 7.185       |              |
| myomeres2_7mm |              | 7    | 2     | f        |         |                |                   | 4     | 37    | 1     | 1      | 33     | 0     | 23    | 99    | 7.082       | 7.120       |              |
| dorsalorgan2_7mm |           | 7    | 3     | f        |         |                |                   | 2     | 20    | 1     | 3      | 53     | 0     | 20    | 99    | 7.062       | 7.142       |              |
| dorsalorgan |             | 7    | 4     | f        |         |                |                   | 4     | 32    | 1     | 0      | 36     | 0     | 27    | 100   | 7.077       | 7.152       |              |
| fossilend_7mm |             | 7    | 5     | f        |         |                |                   | 2     | 23    | 1     | 5      | 51     | 0     | 17    | 99    | 7.085       | 7.119       |              |
| Rank | Model                                                                 | ΔAIC  | Relative likelihood | Akaike weights |
|------|-----------------------------------------------------------------------|-------|---------------------|----------------|
| 1    | Chlorite + Dolomite + Kaolinite + Pyrite                             | 0.000 | 1.000               | 0.255          |
| 2    | Chlorite + Dolomite + Kaolinite + Muscovite + Pyrite + Quartz        | 1.059 | 0.589               | 0.150          |
| 3    | Chlorite + Dolomite + Kaolinite + Muscovite + Pyrite                 | 1.615 | 0.446               | 0.114          |
| 4    | Calcite + Chlorite + Dolomite + Kaolinite + Pyrite                  | 1.741 | 0.419               | 0.107          |
| 5    | Calcite + Chlorite + Dolomite + Kaolinite + Muscovite + Pyrite + Quartz | 1.855 | 0.396               | 0.101          |
| 6    | Chlorite + Dolomite + Kaolinite + Pyrite + Quartz                    | 1.972 | 0.373               | 0.095          |
| 7    | Calcite + Chlorite + Dolomite + Kaolinite + Muscovite + Pyrite       | 3.208 | 0.201               | 0.051          |
| 8    | Calcite + Chlorite + Dolomite + Kaolinite + Pyrite + Quartz         | 3.697 | 0.157               | 0.040          |
| 9    | Chlorite + Kaolinite + Muscovite + Pyrite + Quartz                  | 5.712 | 0.057               | 0.015          |
| 10   | Chlorite + Kaolinite + Pyrite                                        | 6.234 | 0.044               | 0.011          |
| 11   | Chlorite + Kaolinite + Muscovite + Pyrite                           | 6.807 | 0.033               | 0.008          |
| 12   | Dolomite + Kaolinite + Muscovite + Pyrite + Quartz                  | 6.820 | 0.033               | 0.008          |
| 13   | Chlorite + Dolomite + Muscovite + Pyrite + Quartz                   | 7.145 | 0.028               | 0.007          |
| 14   | Calcite + Chlorite + Dolomite + Muscovite + Pyrite + Quartz         | 7.287 | 0.026               | 0.007          |
| 15   | Calcite + Chlorite + Kaolinite + Muscovite + Pyrite + Quartz        | 7.331 | 0.026               | 0.007          |
| 16   | Chlorite + Kaolinite + Pyrite + Quartz                              | 7.831 | 0.020               | 0.005          |
| 17   | Calcite + Chlorite + Kaolinite + Pyrite                             | 8.234 | 0.016               | 0.004          |
| 18   | Calcite + Dolomite + Kaolinite + Muscovite + Pyrite + Quartz        | 8.703 | 0.013               | 0.003          |
| 19   | Calcite + Chlorite + Kaolinite + Muscovite + Pyrite                 | 8.783 | 0.012               | 0.003          |
| 20   | Calcite + Chlorite + Kaolinite + Pyrite + Quartz                    | 9.839 | 0.007               | 0.002          |
| 21   | Kaolinite + Muscovite + Pyrite + Quartz                             | 11.400| 3.35E-03             | 8.53E-04       |
| 22   | Dolomite + Kaolinite + Pyrite                                       | 12.266| 2.17E-03             | 5.53E-04       |
| 23   | Calcite + Dolomite + Kaolinite + Pyrite                             | 12.358| 2.07E-03             | 5.28E-04       |
| 24   | Dolomite + Kaolinite + Pyrite + Quartz                              | 12.534| 1.90E-03             | 4.84E-04       |
| 25   | Calcite + Dolomite + Kaolinite + Pyrite + Quartz                    | 12.602| 1.83E-03             | 4.68E-04       |
| 26   | Kaolinite + Pyrite                                                  | 12.678| 1.77E-03             | 4.50E-04       |
| 27   | Kaolinite + Pyrite + Quartz                                         | 12.725| 1.72E-03             | 4.40E-04       |
| 28   | Dolomite + Kaolinite + Muscovite + Pyrite                           | 13.026| 1.48E-03             | 3.78E-04       |
| 29   | Calcite + Kaolinite + Muscovite + Pyrite + Quartz                   | 13.404| 1.23E-03             | 3.13E-04       |
| 30   | Chlorite + Muscovite + Pyrite                                       | 13.424| 1.22E-03             | 3.10E-04       |
| 31   | Calcite + Dolomite + Kaolinite + Muscovite + Pyrite                 | 13.780| 1.02E-03             | 2.59E-04       |
| 32   | Calcite + Kaolinite + Pyrite + Quartz                               | 13.996| 9.13E-04             | 2.33E-04       |
| 33   | Calcite + Kaolinite + Pyrite                                        | 14.011| 9.07E-04             | 2.31E-04       |
| 34   | Calcite + Chlorite + Muscovite + Pyrite + Quartz                    | 14.333| 7.72E-04             | 1.97E-04       |
| 35   | Kaolinite + Muscovite + Pyrite + Quartz                             | 14.455| 7.26E-04             | 1.85E-04       |
| 36   | Chlorite + Dolomite + Kaolinite                                     | 15.421| 4.48E-04             | 1.14E-04       |
| 37   | Chlorite + Dolomite + Kaolinite + Muscovite + Quartz                | 15.869| 3.58E-04             | 9.13E-05       |
| 38   | Calcite + Kaolinite + Muscovite + Pyrite                            | 15.971| 3.40E-04             | 8.67E-05       |
| 39   | Chlorite + Dolomite + Kaolinite + Muscovite                         | 16.592| 2.49E-04             | 6.36E-05       |
| 40   | Calcite + Chlorite + Dolomite + Kaolinite + Muscovite + Quartz      | 17.029| 2.01E-04             | 5.11E-05       |
| 41   | Calcite + Dolomite + Kaolinite + Quartz                             | 17.266| 1.78E-04             | 4.54E-05       |
| 42   | Calcite + Chlorite + Dolomite + Kaolinite                           | 17.287| 1.76E-04             | 4.49E-05       |
| 43   | Calcite + Chlorite + Dolomite + Kaolinite + Muscovite               | 18.334| 1.04E-04             | 2.66E-05       |
| 44   | Calcite + Chlorite + Dolomite + Kaolinite + Quartz                  | 19.116| 7.07E-05             | 1.80E-05       |
| 45   | Chlorite + Dolomite + Muscovite + Quartz                            | 20.372| 3.77E-05             | 9.61E-06       |
| 46   | Calcite + Chlorite + Dolomite + Muscovite + Quartz                  | 20.803| 3.04E-05             | 7.75E-06       |
| 47   | Dolomite + Kaolinite + Muscovite + Quartz                           | 21.247| 2.43E-05             | 6.20E-06       |
| 48   | Chlorite + Kaolinite + Muscovite + Quartz                           | 21.964| 1.70E-05             | 4.33E-06       |
| 49   | Dolomite + Kaolinite + Quartz                                       | 23.107| 9.60E-06             | 2.45E-06       |
| 50   | Calcite + Dolomite + Kaolinite + Muscovite + Quartz                 | 23.123| 9.33E-06             | 2.43E-06       |
| 51   | Chlorite + Kaolinite + Muscovite                                   | 23.351| 8.50E-06             | 2.17E-06       |
| 52   | Dolomite + Kaolinite + Quartz                                       | 23.365| 8.44E-06             | 2.15E-06       |
| Rank | Model                                                                 | $\Delta$AIC | Relative likelihood | Akaike weights |
|------|-----------------------------------------------------------------------|-------------|---------------------|----------------|
| 53   | Chlorite + Kaolinite                                                  | 23.663      | 7.27E-06            | 1.85E-06       |
| 54   | Calcite + Chlorite + Kaolinite + Muscovite + Quartz                  | 23.869      | 6.56E-06            | 1.67E-06       |
| 55   | Calcite + Dolomite + Kaolinite                                       | 23.964      | 6.26E-06            | 1.59E-06       |
| 56   | Calcite + Dolomite + Kaolinite + Quartz                              | 24.248      | 5.43E-06            | 1.38E-06       |
| 57   | Dolomite + Kaolinite + Muscovite                                     | 24.758      | 4.21E-06            | 1.07E-06       |
| 58   | Chlorite + Kaolinite + Quartz                                        | 24.868      | 3.98E-06            | 1.01E-06       |
| 59   | Calcite + Chlorite + Kaolinite + Muscovite                           | 25.339      | 3.14E-06            | 8.02E-07       |
| 60   | Calcite + Chlorite + Kaolinite                                       | 25.492      | 2.91E-06            | 7.43E-07       |
| 61   | Kaolinite + Quartz                                                   | 25.771      | 2.53E-06            | 6.46E-07       |
| 62   | Kaolinite                                                            | 25.792      | 2.51E-06            | 6.39E-07       |
| 63   | Calcite + Dolomite + Kaolinite + Muscovite                           | 25.847      | 2.44E-06            | 6.22E-07       |
| 64   | Calcite + Chlorite + Kaolinite + Quartz                              | 26.760      | 1.55E-06            | 3.94E-07       |
| 65   | Kaolinite + Muscovite + Quartz                                       | 27.026      | 1.35E-06            | 3.45E-07       |
| 66   | Calcite + Kaolinite + Quartz                                         | 27.695      | 9.68E-07            | 2.47E-07       |
| 67   | Calcite + Kaolinite                                                   | 27.722      | 9.55E-07            | 2.44E-07       |
| 68   | Kaolinite + Muscovite                                                 | 27.733      | 9.50E-07            | 2.42E-07       |
| 69   | Chlorite + Muscovite + Quartz                                        | 27.876      | 8.85E-07            | 2.26E-07       |
| 70   | Chlorite + Dolomite + Muscovite + Pyrite                             | 28.200      | 7.53E-07            | 1.92E-07       |
| 71   | Calcite + Kaolinite + Muscovite + Quartz                             | 29.019      | 5.00E-07            | 1.27E-07       |
| 72   | Calcite + Chlorite + Muscovite + Quartz                              | 29.208      | 4.55E-07            | 1.16E-07       |
| 73   | Calcite + Kaolinite + Muscovite                                      | 29.598      | 3.74E-07            | 9.53E-08       |
| 74   | Calcite + Chlorite + Dolomite + Muscovite + Pyrite                   | 30.193      | 2.78E-07            | 7.08E-08       |
| 75   | Chlorite + Muscovite + Pyrite                                       | 34.965      | 2.56E-08            | 6.51E-09       |
| 76   | Chlorite + Dolomite + Pyrite                                         | 35.107      | 2.38E-08            | 6.07E-09       |
| 77   | Calcite + Chlorite + Muscovite + Pyrite                              | 36.831      | 1.01E-08            | 2.56E-09       |
| 78   | Chlorite + Dolomite + Pyrite + Quartz                                | 36.923      | 9.60E-09            | 2.45E-09       |
| 79   | Calcite + Chlorite + Dolomite + Pyrite                               | 36.952      | 9.46E-09            | 2.41E-09       |
| 80   | Calcite + Chlorite + Dolomite + Pyrite + Quartz                      | 38.763      | 3.83E-09            | 9.75E-10       |
| 81   | Chlorite + Dolomite + Muscovite                                      | 40.103      | 1.96E-09            | 4.99E-10       |
| 82   | Calcite + Chlorite + Dolomite + Muscovite + Quartz                   | 42.093      | 7.24E-10            | 1.85E-10       |
| 83   | Chlorite + Pyrite                                                    | 44.104      | 2.65E-10            | 6.75E-11       |
| 84   | Calcite + Chlorite + Pyrite                                          | 45.042      | 1.66E-10            | 4.22E-11       |
| 85   | Chlorite + Pyrite + Quartz                                            | 45.452      | 1.35E-10            | 3.44E-11       |
| 86   | Calcite + Chlorite + Pyrite + Quartz                                 | 46.421      | 8.31E-11            | 2.12E-11       |
| 87   | Dolomite + Pyrite                                                     | 46.456      | 8.17E-11            | 2.08E-11       |
| 88   | Dolomite + Pyrite + Quartz                                           | 46.501      | 7.99E-11            | 2.04E-11       |
| 89   | Dolomite + Muscovite + Pyrite                                        | 47.775      | 4.22E-11            | 1.08E-11       |
| 90   | Calcite + Dolomite + Pyrite                                          | 47.972      | 3.83E-11            | 9.76E-12       |
| 91   | Calcite + Dolomite + Pyrite + Quartz                                  | 48.109      | 3.57E-11            | 9.11E-12       |
| 92   | Chlorite + Dolomite                                                  | 48.322      | 3.21E-11            | 8.19E-12       |
| 93   | Dolomite + Muscovite + Pyrite + Quartz                               | 48.503      | 2.94E-11            | 7.48E-12       |
| 94   | Pyrite + Quartz                                                      | 48.745      | 2.60E-11            | 6.63E-12       |
| 95   | Pyrite                                                                | 48.828      | 2.50E-11            | 6.36E-12       |
| 96   | Calcite + Dolomite + Muscovite + Pyrite                              | 48.844      | 2.48E-11            | 6.31E-12       |
| 97   | Muscovite + Pyrite                                                   | 48.903      | 2.40E-11            | 6.13E-12       |
| 98   | Chlorite + Muscovite                                                  | 49.134      | 2.14E-11            | 5.46E-12       |
| 99   | Calcite + Dolomite + Muscovite + Pyrite + Quartz                      | 50.040      | 1.36E-11            | 3.47E-12       |
| 100  | Chlorite + Dolomite + Quartz                                         | 50.139      | 1.30E-11            | 3.30E-12       |
| 101  | Calcite + Chlorite + Dolomite                                       | 50.186      | 1.27E-11            | 3.23E-12       |
| 102  | Muscovite + Pyrite + Quartz                                          | 50.268      | 1.21E-11            | 3.10E-12       |
| 103  | Calcite + Muscovite + Pyrite                                         | 50.598      | 1.03E-11            | 2.63E-12       |
| 104  | Calcite + Pyrite + Quartz                                            | 50.745      | 9.57E-12            | 2.44E-12       |
| 105  | Calcite + Pyrite                                                      | 50.828      | 9.18E-12            | 2.34E-12       |
| Rank | Model                                      | ΔAIC  | Relative likelihood | Akaike weights |
|------|-------------------------------------------|-------|---------------------|----------------|
| 106  | Calcite + Chlorite + Muscovite            | 50.922| 8.76E-12            | 2.23E-12       |
| 107  | Calcite + Chlorite + Dolomite + Quartz    | 51.997| 5.12E-12            | 1.30E-12       |
| 108  | Calcite + Muscovite + Pyrite + Quartz     | 52.159| 4.72E-12            | 1.20E-12       |
| 109  | Dolomite                                  | 56.227| 6.17E-13            | 1.57E-13       |
| 110  | Dolomite + Quartz                         | 56.581| 5.17E-13            | 1.32E-13       |
| 111  | Dolomite + Muscovite                      | 56.616| 5.08E-13            | 1.30E-13       |
| 112  | Calcite + Dolomite + Muscovite            | 57.821| 2.78E-13            | 7.09E-14       |
| 113  | Calcite + Dolomite                        | 57.951| 2.61E-13            | 6.64E-14       |
| 114  | Dolomite + Muscovite + Quartz             | 58.153| 2.36E-13            | 6.01E-14       |
| 115  | Calcite + Dolomite + Quartz               | 58.376| 2.11E-13            | 5.37E-14       |
| 116  | Calcite + Dolomite + Muscovite + Quartz   | 59.594| 1.15E-13            | 2.92E-14       |
| 117  | Muscovite                                 | 59.608| 1.14E-13            | 2.90E-14       |
| 118  | Chlorite                                  | 61.139| 5.29E-14            | 1.35E-14       |
| 119  | Calcite + Muscovite                       | 61.495| 4.43E-14            | 1.13E-14       |
| 120  | Muscovite + Quartz                        | 61.510| 4.40E-14            | 1.12E-14       |
| 121  | Calcite + Chlorite                        | 61.564| 4.28E-14            | 1.09E-14       |
| 122  | Chlorite + Quartz                         | 62.106| 3.27E-14            | 8.32E-15       |
| 123  | Quartz                                    | 62.108| 3.26E-14            | 8.31E-15       |
| 124  | Intercept only                            | 62.111| 3.26E-14            | 8.30E-15       |
| 125  | Calcite + Chlorite + Quartz               | 62.638| 2.50E-14            | 6.38E-15       |
| 126  | Calcite + Muscovite + Quartz              | 63.441| 1.67E-14            | 4.27E-15       |
| 127  | Calcite + Quartz                          | 63.843| 1.37E-14            | 3.49E-15       |
| 128  | Calcite                                   | 63.896| 1.33E-14            | 3.40E-15       |
Table S3. Coefficient estimates and confidence intervals for relative abundance models. Coefficient estimates (logit scale) and confidence intervals (CI) for each predictor in the 20 models, with selected-area type (fossil versus matrix) as response. Models were built on 147 measurements for 15 rock/fossil samples based on the Highscore data. Confidence intervals inclusive of zero are in bold.

| Rank | Predictor | Estimate | 95% CI          |
|------|-----------|----------|-----------------|
| 1    | (Intercept) | 2.312    | (0.503, 5.263)  |
|      | Chlorite  | -8.484   | (-17.739, -4.164) |
|      | Dolomite  | 18.973   | (6.518, 39.040)  |
|      | Kaolinite | 13.780   | (9.625, 31.888)  |
|      | Pyrite    | 29.912   | (16.407, 258.236) |
| 2    | (Intercept) | 28.193   | (-8.827, 81.823) |
|      | Chlorite  | -21.251  | (-50.644, -4.699) |
|      | Dolomite  | 18.061   | (5.475, 44.968)  |
|      | Kaolinite | 10.237   | (2.580, 30.468)  |
|      | Muscovite | -16.018  | (-48.649, 6.410) |
|      | Pyrite    | 30.561   | (16.805, 274.410) |
|      | Quartz    | -13.460  | (-43.580, 7.703) |
| 3    | (Intercept) | 4.035    | (-1.893, 12.556) |
|      | Calcite   | -1.726   | (-11.221, 8.098) |
|      | Chlorite  | -8.220   | (-16.969, -3.720) |
|      | Dolomite  | 19.554   | (7.446, 42.736)  |
|      | Kaolinite | 13.494   | (9.821, 31.624)  |
|      | Muscovite | -1.600   | (-7.717, 3.884)  |
|      | Pyrite    | 30.262   | (16.993, 144.375) |
| 4    | (Intercept) | 2.555    | (0.615, 5.374)  |
|      | Calcite   | -1.726   | (-11.321, 8.098) |
|      | Chlorite  | -8.220   | (-16.969, -3.720) |
|      | Dolomite  | 19.554   | (7.446, 42.736)  |
|      | Kaolinite | 13.494   | (9.821, 31.624)  |
|      | Pyrite    | 30.262   | (16.993, 144.375) |
|      | Quartz    | -14.259  | (-44.911, 1.765) |
| 5    | (Intercept) | 30.262   | (2.383, 86.242)  |
|      | Calcite   | -4.124   | (-14.840, 5.100) |
|      | Chlorite  | -21.645  | (-50.795, -8.557) |
|      | Dolomite  | 19.263   | (5.934, 41.858)  |
|      | Kaolinite | 10.318   | (2.590, 30.131)  |
|      | Muscovite | -17.340  | (-51.874, 0.554) |
|      | Pyrite    | 31.132   | (17.810, 85.644) |
|      | Quartz    | -14.259  | (-44.911, 1.765) |
| 6    | (Intercept) | 2.084    | (-1.860, 6.511)  |
|      | Chlorite  | -8.378   | (-17.478, -3.940) |
|      | Dolomite  | 18.823   | (7.661, 38.833)  |
|      | Kaolinite | 13.773   | (9.507, 30.852)  |
|      | Pyrite    | 29.911   | (15.766, 262.151) |
|      | Quartz    | 0.370    | (-5.067, 5.924)  |
| 7    | (Intercept) | 4.345    | (-1.486, 11.796) |
|      | Calcite   | -2.234   | (-11.249, 6.514) |
|      | Chlorite  | -9.054   | (-18.559, -5.066) |
|      | Dolomite  | 18.866   | (6.396, 42.831)  |
|      | Kaolinite | 13.546   | (8.954, 29.787)  |
|      | Muscovite | -1.838   | (-8.022, 4.102)  |
|      | Pyrite    | 30.207   | (17.379, 270.236) |
| 8    | (Intercept) | 2.082    | (-1.615, 6.853)  |
|      | Calcite   | -1.778   | (-11.243, 6.821) |
|      | Chlorite  | -8.084   | (-16.443, -3.746) |
|      | Dolomite  | 19.389   | (8.926, 43.068)  |
|      | Kaolinite | 13.948   | (10.012, 29.107)  |
|      | Pyrite    | 30.117   | (18.351, 266.343) |
|      | Quartz    | 0.445    | (-4.734, 6.112)  |
| 9    | (Intercept) | 28.484   | (0.005, 88.103)  |
|      | Chlorite  | -19.119  | (-49.049, -6.828) |
| Rank | Predictor | Estimate | 95% CI          |
|------|-----------|----------|-----------------|
|      | Kaolinite | 11.422   | (2.838, 30.035) |
|      | Muscovite | -16.996  | (-52.105, 0.167) |
|      | Pyrite    | 30.226   | (16.010, 291.454) |
|      | Quartz    | -13.249  | (-47.813, 4.155) |
| 10   | (Intercept)| 1.602    | (0.057, 4.041)  |
|      | Chlorite  | -5.658   | (-11.854, -1.951) |
|      | Kaolinite | 15.031   | (10.249, 32.994) |
|      | Pyrite    | 29.859   | (16.426, 327.862) |
| 11   | (Intercept)| 4.674    | (-0.952, 11.857) |
|      | Chlorite  | -7.232   | (-14.659, 3.507) |
|      | Kaolinite | 14.357   | (9.778, 17.613)  |
|      | Muscovite | -2.817   | (-8.390, 2.756)  |
|      | Pyrite    | 29.806   | (17.153, 273.737) |
| 12   | (Intercept)| -12.517  | (-25.313, -0.000) |
|      | Dolomite  | 16.856   | (3.908, 36.559)  |
|      | Kaolinite | 15.472   | (11.254, 31.360) |
|      | Muscovite | 8.180    | (2.055, 17.443)  |
|      | Pyrite    | 28.524   | (15.618, 32.989) |
|      | Quartz    | 8.674    | (2.721, 18.817)  |
| 13   | (Intercept)| 55.797   | (37.208, 113.681) |
|      | Chlorite  | -35.263  | (-67.157, -24.383) |
|      | Dolomite  | 18.966   | (6.622, 42.190)  |
|      | Muscovite | -32.828  | (-66.519, -21.863) |
|      | Pyrite    | 29.469   | (15.308, 48.178) |
|      | Quartz    | -27.477  | (-57.716, -1.785) |
| 14   | (Intercept)| 61.553   | (41.833, 127.203) |
|      | Calcite   | -5.444   | (-18.075, 3.056) |
|      | Chlorite  | -36.967  | (-65.463, -25.885) |
|      | Dolomite  | 20.083   | (8.462, 44.178)  |
|      | Muscovite | -36.331  | (-68.031, -24.015) |
|      | Pyrite    | 30.129   | (16.469, 48.178) |
|      | Quartz    | -30.542  | (-59.002, -18.973) |
| 15   | (Intercept)| 30.214   | (0.150, 102.204) |
|      | Calcite   | -2.047   | (-12.151, 6.248) |
|      | Chlorite  | -19.597  | (-54.710, -5.075) |
|      | Kaolinite | 11.453   | (2.780, 25.988)  |
|      | Muscovite | -18.100  | (-61.717, 18.517) |
|      | Pyrite    | 30.599   | (16.909, 257.579) |
|      | Quartz    | -14.019  | (-54.821, 2.693) |
| 16   | (Intercept)| 0.769    | (-2.380, 3.988)  |
|      | Chlorite  | -5.333   | (-11.698, -1.794) |
|      | Kaolinite | 15.009   | (9.961, 28.899)  |
|      | Pyrite    | 29.834   | (16.584, 289.810) |
|      | Quartz    | 1.376    | (-3.453, 6.272)  |
| 17   | (Intercept)| 1.592    | (-0.014, 4.008)  |
|      | Calcite   | 0.572    | (-6.492, 7.607)  |
|      | Chlorite  | -5.766   | (-12.921, -2.626) |
|      | Kaolinite | 14.956   | (10.074, 33.170) |
|      | Pyrite    | 29.763   | (17.623, 263.194) |
| 18   | (Intercept)| -11.941  | (-27.978, -4.393) |
|      | Calcite   | -1.106   | (-9.861, 8.383)  |
|      | Dolomite  | 17.059   | (4.375, 39.347)  |
|      | Kaolinite | 15.473   | (11.640, 31.041) |
|      | Muscovite | 7.807    | (2.014, 19.625)  |
|      | Pyrite    | 28.591   | (16.522, 267.882) |
| Rank | Predictor | Estimate | 95% CI       |
|------|-----------|----------|--------------|
| 19   | Quartz    | 8.379    | (2.577, 18.677) |
|      | Calcite   | -2.047   | (-13.054, 7.228) |
|      | Chlorite  | -19.597  | (-55.360, -5.619) |
|      | Kaolinite | 11.453   | (1.370, 26.587) |
|      | Muscovite | -18.100  | (-63.231, -5.561) |
|      | Pyrite    | 30.599   | (17.203, 268.783) |
|      | Quartz    | -14.019  | (-53.271, 3.812) |
| 20   | Quartz    | 8.775    | (-2.552, 4.543)  |
|      | Calcite   | 0.350    | (-7.381, 8.784)  |
|      | Chlorite  | -5.405   | (-12.366, -1.837) |
|      | Kaolinite | 14.963   | (10.418, 32.361) |
|      | Pyrite    | 29.774   | (16.159, 265.572) |
|      | Quartz    | 1.357    | (-3.493, 7.471)  |
### Table S4. Relative performance of mixed-effects models for relative abundance without quartz.

Models predicted selected-area type (fossil versus matrix) based on measures of relative abundance of calcite, dolomite, kaolinite, muscovite, and pyrite. Models were built on 147 measurements for 15 rock/fossil samples based on the Highscore data. Weights are the ratio of ΔAIC from a given model to the sum of ΔAIC values across all candidate models and are interpreted as the probability that a given model is the “best” (minimizes the Kullback–Leibler discrepancy) of the candidate models, given the data. Grey shading represents those models that received non-trivial weight (ΔAIC<10).

| Model | ΔAIC |
|-------|------|
| Chlorite + Dolomite + Kaolinite + Pyrite | 0.000 | 1.000 | 0.458 |
| Chlorite + Dolomite + Kaolinite + Muscovite + Pyrite | 1.615 | 0.446 | 0.204 |
| Calcite + Chlorite + Dolomite + Kaolinite + Pyrite | 1.741 | 0.419 | 0.192 |
| Calcite + Chlorite + Dolomite + Kaolinite + Muscovite + Pyrite | 3.208 | 0.201 | 0.092 |
| Chlorite + Kaolinite + Pyrite | 6.234 | 0.044 | 0.020 |
| Chlorite + Kaolinite + Muscovite + Pyrite | 6.807 | 0.033 | 0.015 |
| Calcite + Chlorite + Kaolinite + Pyrite | 8.234 | 0.016 |
| Chlorite + Chlorite + Kaolinite + Muscovite + Pyrite | 8.783 | 0.012 |
| Dolomite + Kaolinite + Pyrite | 12.266 | 2.17E-03 | 9.94E-04 |
| Calcite + Chlorite + Dolomite + Kaolinite + Pyrite | 12.358 | 2.07E-03 | 9.49E-04 |
| Kaolinite + Pyrite | 12.678 | 1.77E-03 | 8.09E-04 |
| Dolomite + Kaolinite + Muscovite + Pyrite | 13.026 | 1.48E-03 | 6.80E-04 |
| Calcite + Dolomite + Kaolinite + Muscovite + Pyrite | 13.780 | 1.02E-03 | 4.66E-04 |
| Chlorite + Kaolinite + Pyrite | 14.011 | 9.07E-04 | 4.15E-04 |
| Chlorite + Dolomite + Kaolinite | 14.455 | 7.26E-04 | 3.89E-04 |
| Chlorite + Dolomite + Muscovite | 15.421 | 4.84E-04 | 2.05E-04 |
| Calcite + Chlorite + Dolomite + Muscovite + Pyrite | 15.971 | 3.40E-04 | 1.56E-04 |
| Chlorite + Dolomite + Kaolinite + Muscovite | 16.592 | 2.49E-04 | 1.14E-04 |
| Chlorite + Chlorite + Dolomite + Kaolinite | 17.287 | 1.76E-04 | 8.07E-05 |
| Calcite + Chlorite + Dolomite + Kaolinite + Muscovite | 18.334 | 1.04E-04 | 4.78E-05 |
| Dolomite + Kaolinite | 23.107 | 9.60E-06 | 4.40E-06 |
| Chlorite + Kaolinite + Muscovite | 23.351 | 8.50E-06 | 3.89E-06 |
| Chlorite + Kaolinite | 23.663 | 7.27E-06 | 3.33E-06 |
| Calcite + Dolomite + Kaolinite | 23.964 | 6.26E-06 | 2.87E-06 |
| Dolomite + Kaolinite + Muscovite | 24.758 | 4.21E-06 | 1.93E-06 |
| Chlorite + Chlorite + Kaolinite + Muscovite | 25.339 | 3.14E-06 | 1.44E-06 |
| Calcite + Chlorite + Kaolinite | 25.492 | 2.91E-06 | 1.33E-06 |
| Kaolinite | 25.792 | 2.51E-06 | 1.15E-06 |
| Calcite + Dolomite + Kaolinite + Muscovite | 25.847 | 2.44E-06 | 1.12E-06 |
| Calcite + Kaolinite | 27.722 | 9.55E-07 | 4.38E-07 |
| Chlorite + Muscovite | 27.733 | 9.50E-07 | 4.35E-07 |
| Chlorite + Dolomite + Muscovite + Pyrite | 28.200 | 7.53E-07 | 3.45E-07 |
| Chlorite + Kaolinite + Muscovite | 29.598 | 3.74E-07 | 1.71E-07 |
| Calcite + Chlorite + Dolomite + Muscovite + Pyrite | 30.193 | 2.78E-07 | 1.27E-07 |
| Chlorite + Muscovite + Pyrite | 34.965 | 2.56E-08 | 1.17E-08 |
| Chlorite + Dolomite + Pyrite | 35.107 | 2.38E-08 | 1.09E-08 |
| Calcite + Chlorite + Muscovite + Pyrite | 36.531 | 1.01E-08 | 4.60E-09 |
| Chlorite + Chlorite + Dolomite + Pyrite | 36.952 | 9.46E-09 | 4.33E-09 |
| Chlorite + Dolomite + Muscovite | 40.103 | 1.96E-09 | 8.97E-10 |
| Calcite + Chlorite + Dolomite + Muscovite | 42.093 | 7.24E-10 | 3.32E-10 |
| Chlorite + Pyrite | 44.104 | 2.65E-10 | 1.21E-10 |
| Calcite + Chlorite + Pyrite | 45.042 | 1.66E-10 | 7.59E-11 |
| Dolomite + Pyrite | 46.456 | 8.17E-11 | 3.74E-11 |
| Dolomite + Muscovite + Pyrite | 47.775 | 4.22E-11 | 1.93E-11 |
| Calcite + Dolomite + Pyrite | 47.972 | 3.83E-11 | 1.75E-11 |
| Chlorite + Dolomite | 48.322 | 3.21E-11 | 1.47E-11 |
| Pyrite | 48.828 | 2.50E-11 | 1.14E-11 |
| Calcite + Dolomite + Muscovite + Pyrite | 48.844 | 2.48E-11 | 1.13E-11 |
| Muscovite + Pyrite | 48.903 | 2.40E-11 | 1.10E-11 |
| Chlorite + Muscovite | 49.134 | 2.14E-11 | 9.81E-12 |
| Calcite + Chlorite + Dolomite | 50.186 | 1.27E-11 | 5.80E-12 |
| Calcite + Muscovite + Pyrite | 50.598 | 1.03E-11 | 4.72E-12 |
| Chlorite + Pyrite | 50.828 | 9.18E-12 | 4.20E-12 |
| Rank | Model                          | ΔAIC  | Relative likelihood | Akaike weights |
|------|-------------------------------|-------|---------------------|----------------|
| 54   | Calcite + Chlorite + Muscovite| 50.922| 8.76E-12            | 4.01E-12       |
| 55   | Dolomite                      | 56.227| 6.17E-13            | 2.83E-13       |
| 56   | Dolomite + Muscovite          | 56.616| 5.08E-13            | 2.33E-13       |
| 57   | Calcite + Dolomite + Muscovite| 57.821| 2.78E-13            | 1.27E-13       |
| 58   | Calcite + Dolomite            | 57.951| 2.61E-13            | 1.19E-13       |
| 59   | Muscovite                     | 59.608| 1.14E-13            | 5.21E-14       |
| 60   | Chlorite                      | 61.139| 5.29E-14            | 2.42E-14       |
| 61   | Calcite + Muscovite           | 61.495| 4.43E-14            | 2.03E-14       |
| 62   | Calcite + Chlorite            | 61.564| 4.28E-14            | 1.96E-14       |
| 63   | Intercept only                | 62.111| 3.26E-14            | 1.49E-14       |
| 64   | Calcite                       | 63.896| 1.33E-14            | 6.11E-15       |
Table S5. Coefficient estimates and confidence intervals for relative abundance models without quartz. Coefficient estimates (logit scale) and confidence intervals (CI) for each predictor in the 8 models, with selected-area type (fossil versus matrix) as response. Models were built on 147 measurements for 15 rock/fossil samples based on the Highscore data. Confidence intervals inclusive of zero are in bold.

| Rank | Predictor | Estimate | 95% CI          |
|------|-----------|----------|-----------------|
| 1    | (Intercept) | 2.312    | (0.544, 5.278)  |
|      | Chlorite  | -8.484   | (-17.074, -3.810)|
|      | Dolomite  | 18.973   | (7.680, 41.300) |
|      | Kaolinite | 13.780   | (9.515, 29.690) |
|      | Pyrite    | 29.912   | (18.456, 216.645)|
| 2    | (Intercept) | 4.035    | (-1.626, 11.871)|
|      | Chlorite  | -9.280   | (-20.058, -4.865)|
|      | Dolomite  | 18.252   | (7.548, 42.971) |
|      | Kaolinite | 13.379   | (9.034, 33.022) |
|      | Muscovite | -1.600   | (-7.954, 4.344) |
|      | Pyrite    | 29.923   | (17.890, 259.897)|
| 3    | (Intercept) | 2.355    | (0.601, 5.747)  |
|      | Calcite   | -1.726   | (-10.357, 6.758) |
|      | Chlorite  | -8.220   | (-17.294, -3.678)|
|      | Dolomite  | 19.554   | (7.391, 40.998) |
|      | Kaolinite | 13.949   | (9.215, 28.697) |
|      | Muscovite | -1.838   | (-8.123, 3.443) |
|      | Pyrite    | 30.207   | (15.730, 76.346) |
| 4    | (Intercept) | 4.345    | (-1.309, 12.811)|
|      | Calcite   | -2.234   | (-11.386, 6.280) |
|      | Chlorite  | -9.054   | (-18.862, -4.152)|
|      | Dolomite  | 18.866   | (6.024, 44.492) |
|      | Kaolinite | 13.546   | (9.052, 30.909) |
|      | Muscovite | -1.817   | (-8.123, 3.443) |
|      | Pyrite    | 30.207   | (15.730, 76.346) |
| 5    | (Intercept) | 1.602    | (-0.042, 3.795) |
|      | Chlorite  | -5.658   | (-11.548, -1.186)|
|      | Kaolinite | 15.031   | (9.756, 29.252) |
|      | Pyrite    | 29.859   | (16.532, 298.723)|
| 6    | (Intercept) | 4.674    | (-0.495, 12.166)|
|      | Chlorite  | -7.232   | (-14.639, -3.003)|
|      | Kaolinite | 14.357   | (10.042, 31.454) |
|      | Muscovite | -2.817   | (-9.032, 2.468) |
|      | Pyrite    | 29.806   | (18.211, 297.756)|
| 7    | (Intercept) | 1.592    | (-0.080, 3.938) |
|      | Calcite   | 0.572    | (-7.359, 8.997) |
|      | Chlorite  | -5.766   | (-12.596, -1.768)|
|      | Kaolinite | 14.956   | (10.722, 31.382) |
|      | Pyrite    | 29.763   | (18.079, 258.325)|
| 8    | (Intercept) | 4.723    | (-0.483, 13.140)|
|      | Calcite   | -0.329   | (-8.111, 8.498) |
|      | Chlorite  | -7.190   | (-15.933, -2.834)|
|      | Kaolinite | 14.390   | (9.429, 29.435) |
|      | Muscovite | -2.858   | (-9.387, 1.696) |
|      | Pyrite    | 29.863   | (18.825, 297.223)|
Table S6. Relative performance of mixed-effects models for presence/absence. Models predicted selected-area type (fossil versus matrix) based on presence of kaolinite using the Highscore data. Models were built on 147 measurements for 15 rock/fossil samples. Weights are the ratio of ΔAIC from a given model to the sum of ΔAIC values across all candidate models, and are interpreted as the probability that a given model is the “best” (minimizes the Kullback–Leibler discrepancy) of the candidate models, given the data. Grey shading represents those models that received non-trivial weight (ΔAIC<10).

| Data | Rank | Model                                      | ΔAIC | Relative likelihood | Akaike weights |
|------|------|--------------------------------------------|------|---------------------|----------------|
| Highscore | 1    | Kaolinite + Pyrite                         | 0.000| 1.000               | 0.354          |
|       | 2    | Calcite + Kaolinite + Pyrite               | 0.487| 0.784               | 0.278          |
|       | 3    | Calcite + Dolomite + Kaolinite + Pyrite    | 1.200| 0.549               | 0.194          |
|       | 4    | Dolomite + Kaolinite + Pyrite              | 1.526| 0.466               | 0.165          |
|       | 5    | Dolomite + Kaolinite                       | 9.403| 0.009               | 0.003          |
|       | 6    | Kaolinite                                  | 9.632| 0.008               | 0.003          |
|       | 7    | Calcite + Dolomite + Kaolinite             | 10.553| 5.11E-03           | 1.81E-03       |
|       | 8    | Calcite + Kaolinite                        | 11.483| 3.21E-03           | 1.14E-03       |
|       | 9    | Dolomite + Pyrite                          | 40.084| 1.98E-09           | 7.00E-10       |
|       | 10   | Calcite + Dolomite + Pyrite                | 40.693| 1.46E-09           | 5.16E-10       |
|       | 11   | Pyrite                                     | 42.546| 5.77E-10           | 2.04E-10       |
|       | 12   | Calcite + Pyrite                           | 44.325| 2.37E-10           | 8.39E-11       |
|       | 13   | Dolomite                                   | 46.177| 9.39E-11           | 3.33E-11       |
|       | 14   | Calcite + Dolomite                         | 47.568| 4.69E-11           | 1.66E-11       |
|       | 15   | Intercept only                             | 52.766| 3.48E-12           | 1.23E-12       |
|       | 16   | Calcite                                    | 54.703| 1.32E-12           | 4.68E-13       |
Table S7. Coefficient estimates and confidence intervals for presence/absence models. Coefficient estimates (logit scale) and confidence intervals (CI) for the presence of kaolinite and an intercept-only model, with selected-area type (fossil versus matrix) as response. Both the Highscore and Fityk data are presented. Models were built on 147 measurements for 15 rock/fossil samples. Confidence intervals inclusive of zero are in bold.
Table S8. Relative intensities of chlorite 002, 003, 004, and 005 XRD peak intensities for each selected area with iron content calculation. Abbreviations: Pt = part, Cpt = counterpart, Kaol = kaolinite.

| Fossil  | Selected Area | Fig S1–S15 Location | Pt  | Cpt | Fossil/Matrix | Kaol Fityk | Chlorite Peak Relative Intensity | Iron Content Calculation |
|---------|---------------|---------------------|-----|-----|---------------|------------|---------------------------------|--------------------------|
|         |               |                     |     |     |               |            | 002 | 003 | 004 | 005 | 003/005 | D | Structural Amplitude 003 | 003' | (002+004)/003' | y |
| Canada  | matrix1       | m                   |     |     |               |            | 321.5 | 86.3 | 234.4 | 35.7 | 2.4 | 1.4 | 101.2 | 110 | 5.1 | 5 |
| USNM    | matrix2       | m                   |     |     |               |            | 526.2 | 149.2 | 424.0 | 62.7 | 2.4 | 1.4 | 100.8 | 191 | 5.0 | 5 |
| PAL     | matrix3       | m                   |     |     |               |            | 116.7 | 112.0 | 354.7 | 53.2 | 2.1 | 1.8 | 97.4 | 154 | 3.1 | 2 |
| 198723  | body1         | 1       | f    | 7.16 | | | 279.8 | 55.1 | 185.1 | 21.9 | 2.5 | 1.3 | 102.3 | 69 | 6.8 | 8 |
|         | body2         | 2       | f    | 7.18 | | | 313.7 | 76.7 | 230.5 | 34.6 | 2.2 | 1.6 | 98.8 | 102 | 5.3 | 6 |
|         | body3         | 3       | f    | 7.18 | | | 368.4 | 54.4 | 152.3 | 27.1 | 2.0 | 1.9 | 96.1 | 77 | 6.8 | 8 |
|         | body4         | 4       | f    | | | | 314.9 | 28.2 | 149.9 | 16.4 | 1.7 | 2.4 | 91.8 | 44 | 10.7 | 12 |
|         | body5         | 5       | f    | | | | 0.0 | 37.5 | 175.2 | 18.4 | 2.0 | 1.9 | 96.5 | 52 | 3.3 | 2 |
|         | body6         | 6       | f    | | | | 13.0 | 27.7 | 157.4 | 23.1 | 1.2 | 3.5 | 81.9 | 54 | 3.2 | 2 |
| Canada  | matrix1       | a       | m    |     | | | 600.0 | 149.8 | 361.4 | 55.9 | 2.7 | 1.1 | 104.0 | 180 | 5.3 | 6 |
| USNM    | matrix2       | a       | m    |     | | | 379.8 | 95.1 | 396.4 | 61.3 | 1.6 | 2.7 | 89.0 | 156 | 5.0 | 5 |
| PAL     | matrix3       | a       | m    |     | | | 532.0 | 103.5 | 319.0 | 48.7 | 2.1 | 1.8 | 97.7 | 141 | 6.0 | 7 |
| 198724  | matrix4       | a       | m    |     | | | 423.8 | 134.3 | 329.9 | 45.0 | 3.0 | 0.8 | 107.0 | 153 | 4.9 | 5 |
|         | matrix5       | d       | m    |     | | | 431.8 | 158.3 | 446.1 | 64.1 | 2.5 | 1.3 | 101.8 | 199 | 4.4 | 4 |
|         | matrix6       | d       | m    |     | | | 179.9 | 149.3 | 420.4 | 53.9 | 2.8 | 1.0 | 105.0 | 176 | 3.4 | 2 |
|         | matrix7       | d       | m    |     | | | 556.6 | 139.3 | 359.5 | 48.5 | 2.9 | 0.9 | 106.0 | 162 | 5.7 | 6 |
|         | body1         | 1       | a    | 7.17 | | | 646.4 | 366.0 | 154.0 | 21.0 | 17.4 | -4.4 | 155.6 | 197 | 4.1 | 3 |
|         | body2         | 2       | a    | 7.17 | | | 331.7 | 42.0 | 132.5 | 15.9 | 2.6 | 1.1 | 103.7 | 51 | 9.1 | 11 |
|         | body3         | 3       | a    | 7.17 | | | 374.4 | 289.9 | 162.3 | 24.3 | 11.9 | -3.3 | 145.2 | 179 | 3.0 | 1 |
|         | body4         | 4       | d    | 7.17 | | | 0.0 | 23.6 | 142.8 | 22.6 | 1.0 | 3.9 | 78.1 | 50 | 2.8 | 1 |
|         | body5         | 5       | d    | 7.17 | | | 187.6 | 45.5 | 111.8 | 19.0 | 2.4 | 1.4 | 101.0 | 58 | 5.2 | 5 |
| Canada  | matrix1       | m       |     |     | | | 539.6 | 143.0 | 393.6 | 61.6 | 2.3 | 1.5 | 100.1 | 186 | 5.0 | 5 |
| USNM    | matrix2       | m       |     |     | | | 545.8 | 165.9 | 441.7 | 66.0 | 2.5 | 1.3 | 102.3 | 206 | 4.8 | 5 |
| PAL     | matrix3       | m       |     |     | | | 587.8 | 163.7 | 421.2 | 67.2 | 2.4 | 1.4 | 101.4 | 207 | 4.9 | 5 |
| 199758  | edgeofbristles | 1      | m    | 7.17 | | | 158.7 | 66.9 | 261.4 | 45.0 | 1.5 | 2.8 | 87.8 | 113 | 3.7 | 3 |
|         | centre        | 2      | f    | 7.17 | | | 393.7 | 76.4 | 145.6 | 19.3 | 4.0 | -0.1 | 114.8 | 75 | 7.1 | 8 |
|         | bristlesright | 3      | f    | 7.18 | | | 232.4 | 55.7 | 151.0 | 21.7 | 2.6 | 1.2 | 102.9 | 69 | 5.6 | 6 |
|         | rightbristles2 | 4      | f    | 7.17 | | | 369.3 | 107.4 | 285.0 | 43.3 | 2.5 | 1.3 | 101.9 | 135 | 4.9 | 5 |
|         | centre2       | 5      | f    | 7.17 | | | 247.6 | 51.8 | 142.8 | 16.8 | 3.1 | 0.7 | 107.9 | 58 | 6.7 | 8 |
|         | edgeofbristles2 | 6    | f    | 7.17 | | | 236.2 | 41.7 | 120.1 | 17.1 | 2.4 | 1.4 | 101.5 | 53 | 6.8 | 8 |
| Marnella | matrix1   | a        | m    | 0.0 | 0.0 | 581.8 | 104.0 | 0.0 | | | | | | | |
| USNM    | matrix2       | d       | m    |     | | | 508.4 | 298.2 | 788.3 | 117.9 | 2.5 | 1.3 | 102.5 | 370 | 3.5 | 2 |
| PAL     | matrix3       | d       | m    | 433.5 | 226.5 | 609.8 | 94.1 | 2.4 | 1.4 | 101.1 | 289 | 3.6 | 3 |
| 166587  | matrix4       | d       | m    | 29.9 | 69.8 | 663.0 | 122.4 | 0.6 | 5.7 | 61.4 | 241 | 2.9 | 1 |
|         | matrix5       | a       | m    | 113.7 | 266.9 | 602.1 | 108.9 | 2.5 | 1.3 | 101.6 | 337 | 2.1 | 0 |
| Fossil      | Selected Area | Fig S1–S15 Location | Pt Cpt | Fossil/Matrix | Kaol Fityk | Chlorite Peak Relative Intensity | Iron Content Calculation |
|-------------|---------------|---------------------|--------|---------------|------------|---------------------------------|---------------------------|
|             |               |                     |        |               |            | 002    | 003    | 004    | 005    | 003/005 | D      | Structural Amplitude 003 | 003² | (002+004)/003² | y     |
| matrix6     | a             | m                   |        |               |            | 587.9  | 486.9 | 615.4  | 34.3   | 14.2    | -3.8   | 149.9  | 282   | 4.3    | 4     |
| body1       | 1             | a                   | f      |               |            | 360.7  | 200.9 | 541.0  | 106.1  | 1.9     | 2.1    | 94.5   | 293   | 3.1    | 2     |
| body2       | 2             | a                   | f      |               |            | 127.2  | 192.3 | 567.0  | 94.4   | 2.0     | 1.9    | 96.5   | 269   | 2.6    | 1     |
| body3       | 3             | a                   | f      |               |            | 46.7   | 195.6 | 541.5  | 93.2   | 2.1     | 1.8    | 97.3   | 269   | 2.2    | 0     |
| body4       | 4             | a                   | f      |               | 7.18      | 613.6  | 152.9 | 410.3  | 56.8   | 2.7     | 1.1    | 104.2  | 183   | 5.6    | 6     |
| body5       | 5             | d                   | f      |               | 0.0       | 105.9  | 495.8 | 87.2   | 1.2    | 3.4     |        | 82.3   | 204   | 2.4    | 0     |
| body6       | 6             | d                   | f      |               | 0.0       | 24.8   | 297.6 | 26.6   | 0.9    | 4.2     |        | 75.0   | 57    | 5.2    | 5     |
| body7       | 7             | d                   | f      |               | 0.0       | 0.0    | 0.0   | 61.8   | 0.0    |         |        | 111.8  | 242   | 6.1    | 7     |
| body8       | 8             | d                   | f      |               | 449.4     | 256.2  | 759.1 | 97.5   | 2.6    | 1.1     |        | 103.5  | 311   | 3.9    | 3     |
| body9       | 9             | d                   | f      |               | 1000.0    | 231.9  | 464.8 | 65.4   | 3.5    | 0.3     |        | 111.8  | 242   | 6.1    | 7     |
| Marrella    | matrix1       | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| Marrella    | matrix1       | Port 3              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| USNM        | matrix1       | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| PAL         | matrix3       | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| 229990      | head_scan1    | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| USNM        | matrix1       | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| PAL         | matrix3       | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| 230379      | head_scan1    | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| USNM        | matrix1       | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| PAL         | matrix3       | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| 139217      | body1         | Port 7              | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| body2       | 2             | f                   | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| body3       | 3             | f                   | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| body4       | 4             | f                   | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| body5_12mm  | 5             | f                   | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| body6_12mm  | 6             | f                   | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| body7_22mm  | 7             | f                   | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| body8_22mm  | 8             | f                   | 7.18   | body/center_1 | body/center_1 | 273.7 | 480.5 | 140.5  | 1.2    | 1.8     |        | 107.7  | 311   | 3.9    | 3     |
| Fossil  | Selected Area | Fig S1–S15 Location | Pt Cpt | Fossil/Matrix | Kaolinite Fityk | Chlorite Peak Relative Intensity | Iron Content Calculation |
|---------|----------------|----------------------|--------|---------------|----------------|-------------------------------|------------------------|
| PAL     | matrix3        | m                    | m      | m             | 287.3          | 130.0                         | 128                   |
| 155600  | eyes 12mm      | f                    | f      | f             | 198.8          | 72.4                          | 132                   |
|         | eyesnew 7mm    | 2                    | 7.19   | f             | 313.7          | 64.3                          | 143                   |
|         | claw 22mm      | 3                    | f      | f             | 219.7          | 93.4                          | 148                   |
|         | flapsnew 2_7mm | 4                    | f      | f             | 356.1          | 108.1                         | 140                   |
|         | flapsnew 3_7mm | 4                    | f      | f             | 357.5          | 114.0                         | 137                   |
|         | flapsnew 7mm   | 5                    | f      | f             | 362.9          | 87.4                          | 136                   |
| partial | f             | f                    | f      | f             | 14.6           | 137.2                         | 130                   |
| flaps   | 22mm           | 7                    | f      | f             | 14.3           | 90.0                          | 128                   |
| gut22   | 8              | 7.16                 | f      | f             | 493.5          | 105.7                         | 130                   |
| gut     | 9              | f                    | f      | f             | 701.7          | 77.5                          | 132                   |
| gutnew 12mm | 10          | f                    | f      | f             | 210.6          | 74.6                          | 132                   |
| gut3_22mm | 11           | f                    | f      | f             | 346.6          | 102.3                         | 127                   |
| gutnew 2_7mm | 12           | f                    | f      | f             | 262.9          | 66.1                          | 129                   |
| Ottoia  | matrix         | m                    | m      | m             | 311.4          | 67.2                          | 115                   |
| USNM    | matrix2        | m                    | m      | m             | 160.7          | 99.3                          | 114                   |
| PAL     | matrix3        | m                    | m      | m             | 0.0            | 26.8                          | 111                   |
| 188616  | gut2           | m                    | m      | m             | 246.8          | 79.4                          | 119                   |
| gutend 7mm | 1             | f                    | f      | f             | 253.7          | 78.1                          | 116                   |
| gut     | 2              | f                    | f      | f             | 56.4           | 58.0                          | 117                   |
| gut3_7mm | 3             | f                    | f      | f             | 134.6          | 59.2                          | 118                   |
| body2_7mm | 4             | f                    | f      | f             | 52.1           | 55.2                          | 119                   |
| Ottoia  | matrix         | m                    | m      | m             | 1000.0         | 236.9                         | 115                   |
| USNM    | matrix2        | m                    | m      | m             | 30.8           | 191.3                         | 116                   |
| PAL     | matrix3        | m                    | m      | m             | 182.8          | 130.2                         | 117                   |
| 188617  | body3_7mm      | 1                    | f      | f             | 805.5          | 255.5                         | 118                   |
| gut     | 2              | f                    | f      | f             | 839.9          | 243.9                         | 119                   |
| body    | 3              | f                    | f      | f             | 883.2          | 270.6                         | 118                   |
| body2_7mm | 4             | f                    | f      | f             | 601.4          | 184.5                         | 117                   |
| Ottoia  | matrix1        | m                    | m      | m             | 541.6          | 138.2                         | 112                   |
| USNM    | matrix2        | m                    | m      | m             | 464.6          | 133.5                         | 111                   |
| PAL     | matrix3        | m                    | m      | m             | 7.18           | 146.2                         | 110                   |
| 198565  | backbody1      | 1                    | f      | f             | 165.0          | 87.0                          | 116                   |
| gut     | 2              | f                    | f      | f             | 328.2          | 118.8                         | 115                   |
| backbody2 | 3             | f                    | f      | f             | 193.8          | 93.3                          | 113                   |
| Fossil | Selected Area | Fig S1–S15 Location | Pt Cpt | Fossil/Matrix | Kaol Fityk | Chlorite Peak Relative Intensity | Iron Content Calculation |
|--------|---------------|----------------------|-------|--------------|------------|---------------------------------|--------------------------|
|        |               |                      |       |              |            | 002 | 003 | 004 | 005 | 003/005 | D | Structural Amplitude 003 | 003^3 | (002+004)/003^3 | y |
| Ottoia | matrix1       | m                    | 446.7 | 129.1        | 579.9      | 92.0 | 1.4 | 3.0 | 86.2 | 226 | 4.5 | 4 |
| USNM   | matrix2       | m                    | 539.8 | 117.0        | 482.8      | 80.8 | 1.4 | 2.9 | 87.1 | 201 | 5.1 | 5 |
| PAL    | matrix3       | m                    | 508.1 | 145.9        | 410.4      | 92.6 | 1.6 | 2.7 | 89.4 | 238 | 3.9 | 3 |
| 198577 | body1         | 1                    | 719.0 | 329.8        | 331.9      | 55.4 | 6.0 | -1.3 | 126.0 | 270 | 3.9 | 3 |
|        | body2         | 2                    | 581.2 | 115.3        | 241.2      | 27.8 | 4.1 | -0.2 | 116.1 | 111 | 7.4 | 9 |
| 198688 | body3         | 3                    | 445.8 | 132.6        | 295.4      | 70.1 | 1.9 | 2.1 | 94.5 | 193 | 3.8 | 3 |
|        | body4         | 4                    | 630.8 | 89.1         | 54.3       | 23.0 | 3.9 | 0.0 | 114.2 | 89  | 7.7 | 9 |
|        | body5         | 5                    | 472.4 | 138.8        | 399.9      | 55.8 | 2.5 | 1.3 | 102.0 | 174 | 5.0 | 5 |
|        | body6         | 6                    | 781.1 | 96.7         | 443.7      | 40.9 | 2.4 | 1.5 | 100.6 | 124 | 9.8 | 12 |
|        | body7         | 7                    | 348.4 | 104.2        | 289.5      | 71.0 | 1.5 | 2.9 | 87.5 | 117 | 3.6 | 3 |
| Pikaia | matrix1       | a                    | 776.0 | 189.6        | 497.9      | 72.2 | 2.6 | 1.1 | 103.5 | 230 | 5.5 | 6 |
| USNM   | matrix2       | a                    | 411.2 | 159.6        | 472.8      | 84.2 | 1.9 | 2.1 | 94.5 | 233 | 3.8 | 3 |
| PAL    | matrix3       | a                    | 692.4 | 198.8        | 520.6      | 78.7 | 2.5 | 1.3 | 102.4 | 247 | 4.9 | 5 |
| 198692 | matrix4       | d                    | 594.8 | 157.9        | 444.9      | 72.6 | 2.2 | 1.7 | 98.3 | 213 | 4.9 | 5 |
|        | matrix5       | d                    | 736.1 | 197.3        | 480.9      | 69.7 | 2.8 | 0.9 | 105.6 | 231 | 5.3 | 5 |
|        | matrix6       | d                    | 671.3 | 209.0        | 536.1      | 81.7 | 2.6 | 1.2 | 102.8 | 258 | 4.7 | 4 |
|        | body1         | 1                    | 0.0   | 111.6        | 349.4      | 52.3 | 2.1 | 1.8 | 97.8 | 152 | 2.3 | 0 |
|        | body2         | 2                    | 0.0   | 40.1         | 326.1      | 48.0 | 0.8 | 4.5 | 72.0 | 101 | 3.2 | 2 |
|        | body3         | 3                    | 253.0 | 146.8        | 430.1      | 65.6 | 2.2 | 1.6 | 99.1 | 195 | 3.5 | 2 |
|        | body4         | 4                    | 131.6 | 144.3        | 471.7      | 81.1 | 1.8 | 2.3 | 92.8 | 218 | 2.8 | 1 |
|        | body5         | 5                    | 174.8 | 78.3         | 383.5      | 61.8 | 1.3 | 3.3 | 83.4 | 146 | 3.8 | 3 |
|        | body6         | 6                    | 765.5 | 140.8        | 258.8      | 43.6 | 3.2 | 0.5 | 109.2 | 154 | 6.7 | 8 |
|        | body7         | 7                    | 224.5 | 96.2         | 285.1      | 64.2 | 1.5 | 2.8 | 88.0 | 162 | 3.2 | 2 |
|        | body8         | 8                    | 607.0 | 178.2        | 466.5      | 64.4 | 2.8 | 1.0 | 104.9 | 211 | 5.1 | 5 |
|        | body9         | 9                    | 381.7 | 117.0        | 363.6      | 60.6 | 1.9 | 2.1 | 95.0 | 169 | 4.4 | 4 |
| Pikaia | matrix1       | m                    | 875.6 | 274.1        | 778.4      | 112.0 | 2.4 | 1.4 | 101.6 | 346 | 4.8 | 5 |
| USNM   | matrix2       | m                    | 1000.0| 284.2        | 782.3      | 116.3 | 2.4 | 1.4 | 101.5 | 359 | 5.0 | 5 |
| PAL    | matrix3       | m                    | 1000.0| 281.5        | 753.4      | 104.0 | 2.7 | 1.1 | 104.3 | 337 | 5.2 | 5 |
| 198692 | body1         | 1                    | 743.0 | 160.2        | 416.8      | 100.8 | 1.6 | 2.6 | 89.7 | 259 | 4.5 | 4 |
|        | body2         | 2                    | 574.8 | 248.0        | 671.0      | 101.6 | 2.4 | 1.4 | 101.5 | 314 | 4.0 | 3 |
|        | body3         | 3                    | 427.7 | 172.6        | 524.8      | 90.7 | 1.9 | 2.1 | 94.6 | 251 | 3.8 | 3 |
|        | body4         | 4                    | 1000.0| 294.6        | 715.7      | 104.9 | 2.8 | 0.9 | 105.3 | 346 | 5.0 | 5 |
| Pikaia | matrix        | m                    | 1000.0| 395.0        | 991.1      | 142.5 | 2.8 | 1.0 | 105.0 | 467 | 4.3 | 4 |
| USNM   | matrix3       | m                    | 714.8 | 314.8        | 817.5      | 128.0 | 2.5 | 1.3 | 101.7 | 396 | 3.9 | 3 |
| PAL    | matrix4       | m                    | 718.0 | 258.4        | 719.4      | 140.7 | 1.8 | 2.2 | 93.6 | 384 | 2.3 | 0 |
| 202220 | myomeres      | 1                    | 355.3 | 168.3        | 622.1      | 108.1 | 1.6 | 2.7 | 89.1 | 276 | 3.5 | 2 |
| Fossil          | Selected Area | Fig S1–S15 Location | Pt Cpt | Fossil/Matrix | Kaol Fityk | Chlorite Peak Relative Intensity | Iron Content Calculation |
|-----------------|---------------|---------------------|--------|---------------|------------|----------------------------------|--------------------------|
|                 |               |                     |        |               | 002 | 003 | 004 | 005 | 003/005 | D | Structural Amplitude 003 | 003' | (002+004)/003' | y  |
| myomeres2_7mm   | 2             | f                   |        |               | 503.6 | 311.2 | 865.8 | 126.7 | 2.5 | 1.3 | 101.7 | 392 | 3.5 | 2  |
| dorsalorgan2_7mm| 3             | f                   |        |               | 910.3 | 264.0 | 741.5 | 109.4 | 2.4 | 1.4 | 101.2 | 336 | 4.9 | 5  |
| dorsalorgan     | 4             | f                   |        |               | 797.1 | 271.9 | 784.1 | 140.2 | 1.9 | 2.0 | 95.1  | 391 | 4.0 | 3  |
| fossilend_7mm   | 5             | f                   |        |               | 861.8 | 302.4 | 940.6 | 21.9  | 13.8 | -3.8| 149.2 | 177 | 10.2| 12 |
Figure S1. *Canadia spinosa* USNM PAL 198723. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Oxford.
Figure S2. *Canadia spinosa* USNM PAL 198724 with part and counterpart. A, D: Light image showing locations for selected-area XRD. B, E: SEM-EDS map, Al (red) C (blue) Si (green). C, F: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Scales in E and F same as in D. Data collected at the University of Oxford.
Figure S3. *Canadia spinosa* USNM PAL 199758. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Bristol.
Figure S4. *Marrella splendens* USNM PAL 166587 with part and counterpart. A, D: Light image showing locations for selected-area XRD. B, E: SEM-EDS map, Al (red) C (blue) Si (green). C, F: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Scales in E and F same as in D. Data collected at the University of Oxford.
Figure S5. *Marrella splendens* USNM PAL 229990. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Bristol.
Figure S6. *Marella splendens* USNM PAL 230379. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Bristol.
Figure S7. *Opabina regalis* USNM PAL 139217. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Oxford.
Figure S8. *Opabinia regalis* USNM PAL 155600. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Bristol.
Figure S9. *Ottoia prolifica* USNM PAL 188616. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Bristol.
Figure S10. *Ottoia prolifica* USNM PAL 188617. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Bristol.
Figure S11. *Ottoia prolifica* USNM PAL 198565. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Oxford.
Figure S12. *Ottoia prolifica* USNM PAL 198577. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Oxford.
Figure S13. *Pikaia gracilens* USNM PAL 198688 with part and counterpart. A, D: Light image showing locations for selected-area XRD. B, E: SEM-EDS map, Al (red) C (blue) Si (green). C, F: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Scales in E and F same as in D. Data collected at the University of Oxford.
Figure S14. *Pikaia gracilens* USNM PAL 198692. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Oxford.
Figures S15. *Pikaia gracilens* USNM PAL 202220. A: Light image showing locations for selected-area XRD. B: SEM-EDS map, Al (red) C (blue) Si (green). C: SEM-EDS map, Ca (magenta) Fe (cyan) P (yellow). Scales in B and C same as in A. Data collected at the University of Bristol.
Figure S16. Pseudovoigt function maxima in d-spacing, partitioned into three clusters based on parameterized finite Gaussian mixture models. Clusters 1 and 2 represent chlorite, whereas cluster 3 represents kaolinite.
Figure S17. Comparison of chlorite iron content, $y$, between fossil and matrix analyses.