



# Elemental analysis by neutron activation analysis and synchrotron x-ray fluorescence microscopy of ocean plastics ingested by pelagic seabirds

Jennifer L. Lavers<sup>a,b,c,\*</sup> , Nicholas R. Howell<sup>d</sup> , Alexander L. Bond<sup>a,c</sup> , Daryl L. Howard<sup>e</sup> ,  
Martin D. de Jonge<sup>e</sup> , Ljiljana Puskar<sup>e,f</sup> , Richard B. Banati<sup>d,g,h</sup> 

<sup>a</sup> Bird Group, The Natural History Museum, Tring, Hertfordshire HP23 6AP, United Kingdom

<sup>b</sup> Gulbali Institute, Charles Sturt University, Wagga Wagga, New South Wales 2678, Australia

<sup>c</sup> Adrift Lab, Underwood, Tasmania 7268, Australia

<sup>d</sup> Australian Nuclear Science and Technology Organisation (ANSTO), Locked Bag 2001, Kirrawee, New South Wales 2232, Australia

<sup>e</sup> Australian Synchrotron, Australian Nuclear Science and Technology Organisation (ANSTO) Melbourne, 800 Blackburn Road, Clayton, Victoria 3168, Australia

<sup>f</sup> Helmholtz-Zentrum für Materialien und Energie GmbH, Berlin 12489, Germany

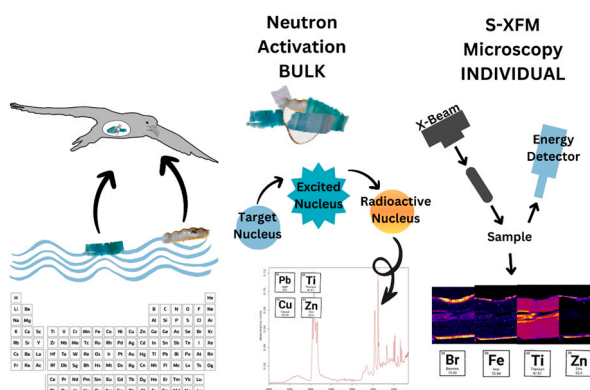
<sup>g</sup> Faculty of Medicine and Health, University of Sydney, Sydney, New South Wales 2006, Australia

<sup>h</sup> Santuario Accademico S. Giovanni D'Andorno, Casa Alpina 'Principessa Laetitia', Frazione Bele, Campiglia Cervo 13812, Italy

## HIGHLIGHTS

- Bulk elemental composition of total plastics ingested by seabirds.
- Individual plastics described using X-ray fluorescence microscopy.
- Plastic biofilm and discolouration associated with higher elemental load.
- Shearwater chicks were mostly fed high density polyethylene and polypropylene.

## GRAPHICAL ABSTRACT



## ARTICLE INFO

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## ABSTRACT

We report the combined use of Neutron Activation Analysis (NAA) for bulk measurement of marine plastics ingested by wildlife, with a more detailed analysis of individual plastics at different stages of degradation using synchrotron X-ray fluorescence microscopy (S-XFM). On average, Sable Shearwaters ( $n = 9$ ) ingested  $4.16 \pm 4.62$  g of plastics ( $50 \pm 35$  items), most of which were high-density polyethylene (47.4 %) and polypropylene (42.6 %) as determined by attenuated total reflectance Fourier transform infrared spectroscopy. Using NAA, the most abundant elements (Ti, Zn, Cd, Cu, Cr, Sr) were those commonly associated with plastic additives that confer UVC resistance, mechanical properties, or colouration. S-XFM revealed that visually and structurally near identical plastics may not only contain different chemical elements, but that the internal spatial distribution of these elements can vary substantially. S-XFM also detected the presence of lead (Pb) which may indicate prior

\* Corresponding author at: Bird Group, The Natural History Museum, Tring, Hertfordshire HP23 6AP, United Kingdom.

E-mail address: [jennifer.lavers1@nhm.ac.uk](mailto:jennifer.lavers1@nhm.ac.uk) (J.L. Lavers).

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recycling history of the plastic feed stock. A consistent finding was the accumulation of iron (Fe) and bromine (Br) at the surface of the degrading plastics, attributable to biofilm formation. Our observations highlight that bird populations ingesting marine plastics are exposed to an unpredictable profile of chemical elements, the degradation-dependent release rate of which is unknown in the acidic and enzymatically-active stomach environment. Based on the variability of their elemental content, we propose to regard marine plastics as 'mixed waste'. We speculate that plastics more generally could be doped with complex elemental 'fingerprints' for the purpose of traceability and establishment of an unbroken chain of custody.

## 1. Introduction

Plastics have revolutionized manufacturing and production in the last 80 years, including more recently making manufacturing widely available to individuals in the form of 3D printers [60]. This underpins an unabated exponential increase in plastic production globally [25,49] and concomitant rapid rise of plastics in the environment where they have become a pervasive threat to ecosystems and species [46] as well as humans [38].

While in virgin condition, most plastics are largely harmless or of low toxicity making them suitable for a wide variety of applications from medicine to food storage [16,23,82], though many remain untested before going to market [83]. The rate of chemical leaching from unadulterated polymers tends to be low and at concentrations that make acute, easily observable adverse health effects unlikely [16,23].

However, when exposed to the environment, notably the harsh conditions of the open seas, plastics enter complex decay pathways and through not yet fully understood processes, cause the release of toxic components, such as hazardous chemicals or metal additives, or metals acquired through adsorptive action during prolonged weathering [3,73]. Weathering itself is a complex process of material transformation that includes mechanical destruction [53], surface oxidation [5], and biofilm growth [4,32,79] that in turn facilitates the sorption of (often hydrophobic) contaminants (e.g., polychlorinated biphenyls (PCBs), polycyclic aromatic hydrocarbons (PAHs), and per- and polyfluoroalkyl substances (PFAS; [14]) from the ambient environment [15,58,59], which can then be transferred to biota (e.g., through ingestion or physical transportation; [11]). The degradation of marine plastics causes physico-chemical changes in surface properties that may affect environmental transport pathways of radionuclides [20,33] that would not be predicted solely based on adsorption studies using virgin plastics [8].

While the compositional heterogeneity, variable nature of use, and degradation-dependent compositional and surface changes have made it difficult to ascertain the health impact of plastics on wildlife [37,42] beyond malnutritional effects there is a growing body of evidence of the physiological impacts related to plastic ingestion even without accounting for the physical properties of the plastics or their associated chemicals [12,18,57]. Correlational analysis of ingested plastics and elemental composition of concurrently grown feathers has suggested some relationships may exist with certain chemical elements [39,40,51], but a more detailed description of the elemental content and its heterogeneity in plastics 'sampled' by wildlife is lacking.

To close the gap between the existing survey studies of marine plastics and the factual uptake in wildlife, specifically in pelagic birds, we examined the entire stomach content of ingested plastics in individual Sable Shearwaters (*Ardenna carneipes*) [10] using attenuated total reflectance Fourier transform infrared (ATR FT-IR) spectroscopy to determine the prevalence of the type of plastics and subsequent the bulk analysis of the elemental composition of the total ingested plastics load using neutron activation analysis (NAA) as well as the 'histology' of individual plastics pieces by synchrotron X-ray fluorescence microscopy (S-XFM) to describe the spatial distribution of chemical elemental within individual plastics fragments.

## 2. Methods

### 2.1. Sample collection

We sampled plastics ingested by Sable Shearwater fledglings on Lord Howe Island, Australia (31.53°S, 159.07°E) from 2011 to 2014. In total, nine birds were captured by hand on the colony surface immediately prior to fledging at ca. 90 days old. During their nest-bound stage, young birds are fed by both parents, who also provision large quantities of plastics [42]. The fledglings' stomachs were flushed with water (for details see [39,41,42]), resulting in the plastics being regurgitated. Pieces were then washed with tap water, dried, and stored individually in aluminium foil.

Three different analytical methods were used:

1. *Attenuated total reflectance Fourier transform infrared (ATR FT-IR) spectroscopy* of each retrieved plastic fragment (in total 448 pieces; mean  $\pm$  SD 49.8 g  $\pm$  34.7 plastics per bird) to estimate the prevalence of various plastic types ingested by our cohort of birds [52].
2. *Neutron activation analysis (NAA)* of the combined cumulative plastics retrieved from the stomachs of eight Sable Shearwater fledglings to obtain an indicative estimate of the concentration of various chemical elements in the ingested plastics [17].
3. *Synchrotron X-ray fluorescence microscopy (S-XFM)* was used on a further set of individual plastic pieces (n = 11) selected from across the different stomach contents to illustrate the presence and spatial distribution of chemical elements typically found individual plastic fragments of different polymer type, colour, and state of degradation [19].

### 2.2. Attenuated total reflectance FT-IR spectroscopy

ATR FT-IR spectroscopy was conducted using a Bruker Alpha spectrometer fitted with a Platinum ATR module to identify the parent polymer composition of plastic items ingested by the shearwaters. This method determines the chemical composition of a sample by directing infrared radiation through a diamond ATR crystal kept in contact with the sample. The high refractive index of the crystal causes total internal reflectance at the crystal-sample interface with some of the light penetrating through the sample. The amount of attenuation of infrared signal is measured following the interaction of the sample with specific wavelengths of light. The molecular structure of the substance is represented by the resulting absorbance spectrum, creating an individual and unique molecular fingerprint of each sample [52].

Plastics from each of the nine birds were analysed individually using ATR FT-IR and the resulting spectra along with information on colour, texture and size were recorded. The oxidation levels of these fragments were assessed by looking at the carbonyl and fingerprint regions of their spectra and used in conjunction with information about colour and texture to estimate exposure to marine conditions. All FT-IR analyses were performed using OPUS (Bruker, version 6.5) and classified after a first pass inspection of the obtained spectrum by similarity search against a database (based on common resin codes) of known polymer spectra (polymer library OPUS 8.5 software (e.g., [76]).

### 2.3. Neutron activation analysis

To determine the type and concentration of chemical elements associated with the plastics load recovered from the stomach of eight different shearwaters, samples were analysed using the NAA facility of the Open Pool Australian Light water (OPAL) reactor at the Australian Nuclear Science and Technology Organization (ANSTO) in Sydney. NAA is a highly sensitive, selective, accurate (95–96 % accuracy) and precise method, capable of multi-element detection (approx. 63 elements, Table S1; [6,26]). For irradiation (i.e., neutron activation) in the reactor, the samples were packed into 1 cm<sup>2</sup> transparent PE boxes.

Following neutron activation, a purpose-designed detector and a computerized data processing system was used to simultaneously measure and interpret the individual energy signals ( $\gamma$  rays), producing a continual real-time emission spectrum from the activated elements that allows the decay measurements of elements with both short (minutes) and longer decay times (hours to days; [2,6]).

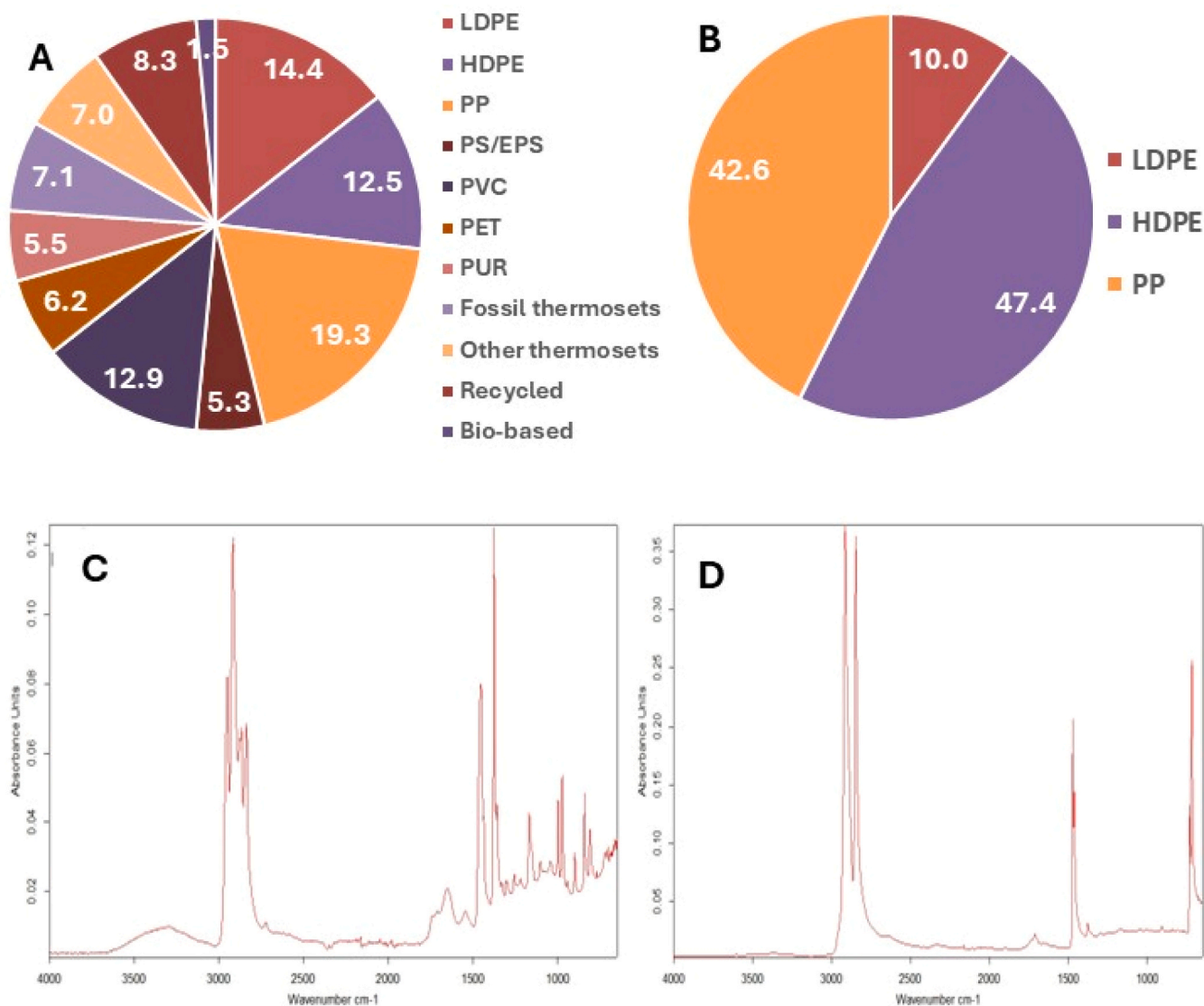
### 2.4. Synchrotron X-ray fluorescence microscopy

Eleven ingested plastic fragments of variable colour and stage of degradation were cut by microtome into 20  $\mu$ m thick sections. X-ray fluorescence spectra were collected on the XFM beamline at the Australian Synchrotron in Melbourne using a 9  $\mu$ m 16.5 keV beam [30]. The beam was scanned across the sample with a step size of 10  $\times$  10  $\mu$ m and dwell time of 4.88 ms. The resulting spectra were collected using the Maia 384 detector array [47,63]. Curve fitting and analysis were performed using GeoPIXE II [64].

## 3. Results

### 3.1. ATR FT-IR spectroscopy

The mass of plastics (a total 448 of pieces; mean  $\pm$  SD 49.8  $\pm$  34.7 fragments per bird) across the nine birds varied from 2.02 to 15.24 g (mean  $\pm$  SD 4.16 g  $\pm$  4.62). By weight, high density polyethylene (HDPE; 47.4 %; Fig. 1B) and polypropylene (PP; 42.6 %) were the most



**Fig. 1.** (A) The 2022 world-wide plastics manufacture as percentage of polymer type ([48]; LDPE low density polyethylene, HDPE high density polyethylene, PP polypropylene, PS/EPS polystyrene, PVC polyvinyl chloride, PET polyethylene terephthalate, PUR polyurethane). (B) Plastics ingested by Sable Shearwater *A. carneipes* fledglings as a percentage weight of polymer type as determined by ATR-FTIR. Example spectra of the two main polymers ingested by shearwater fledglings, (C) polypropylene, and (D) polyethylene, both demonstrating absorption at the C=O stretch (1760–1665 cm<sup>-1</sup>), suggestive of environmental exposure. Axis labels for panels C and D are Wavenumber cm<sup>-1</sup> and Absorbance Units.

ingested polymers, with a smaller fraction of low-density polyethylene (LDPE; 10.0 %). All plastic fragments (LDPE, HDPE, PP) showed significant absorption at the C=O stretch ( $1760\text{--}1665\text{ cm}^{-1}$ ), not present in virgin materials, suggesting substantial environmental exposure (Fig. 1 C, D).

### 3.2. Neutron activation analysis

Bulk NAA of cumulative plastic content taken from eight different Sable Shearwater fledglings revealed a range of chemical elements (Fig. 2). The most abundant elements, also detected by S-XFM (Figs. 3–5), were Ti and Zn as well as Cu, Cr, Sr, Fe, and Br.

### 3.3. Synchrotron X-ray fluorescence microscopy

A selection of 11 different coloured plastics recovered from the stomachs of Sable Shearwater fledglings were studied in detail by synchrotron X-ray fluorescence microscopy. Virgin clear plastics in the form of unprocessed nurdles only contained zinc (Zn) homogeneously distributed through their entire volume, while weathered nurdles were covered by a thin layer of iron (Fe) and bromine (Br; Fig. 3B). In contrast, processed plastics in items, such as bottle caps and fragments from unidentified items, showed a range of additional elements. All white plastics also contained titanium (Ti) as well as variably presented and distributed other elements, such as lead (Pb), strontium (Sr) and chromium (Cr). Weathered surfaces contained Fe and Br (Figs. 3B and 4G), though occasionally Br is found internally (Fig. 4H). Green and blue plastics, in addition to the consistently present Zn and Ti, contained Pb, copper (Cu) and Cr in variable patterns of distribution (Fig. 5).

## 4. Discussion

This study expands on our earlier work [39], and focuses on plastic items ‘sampled’ by wildlife. Sampling ingested plastics from Sable

Shearwaters revealed a relevant cross-section of typical marine plastics (total  $n = 448$  ingested items), and thus a real-life exposure scenario. These plastics were mostly HDPE and polypropylene as determined by FT-IR spectroscopy. While no reliable methodologies exist to determine the duration of outdoor exposure of plastics collected in the field, FT-IR spectroscopy used in conjunction with morphological characteristics (such as colour and texture) can give an indication of the extent of weathering [24,28], from which exposure can be deduced. To do this, the amount of oxidation (caused by weathering) can be assessed by looking at both the intensity of stretching band in the carbonyl region ( $1760\text{--}1665\text{ cm}^{-1}$ ) and the appearance of new stretching bands in the fingerprint region ( $< 1665\text{ cm}^{-1}$ ). Our samples highlighted a pattern of absorption at the C=O stretch ( $1760\text{--}1665\text{ cm}^{-1}$ ) confirming that the ingested plastics had undergone significant weathering.

The combined measurement of the cumulative load of chemical elements (NAA) associated with the ingestion of ocean plastics by pelagic birds with the spatially resolved distribution of chemical elements (S-XFM) in individual plastic fragments revealed the cumulative abundance of chemical elements birds are exposed to (Fig. 2), as well as a previously unreported heterogeneity in the composition and spatial sub-millimetre distribution of chemical elements within individual plastics of apparent macroscopic similarity (Figs. 3–5). The latter suggests that similar appearing plastics hide different chemical element composition, and that internal spatial distribution of these elements will result in differential exposure during the weathering process. While essentially all plastics, including unprocessed clear plastics in the form of nurdles (resin pellets) contained Zn, a common additive, several other elements are present in plastics that hint at different manufacturing process and potentially source of ingredients. Zinc oxide is commonly used as a UV stabilizer, protecting plastic products from degradation caused by ultraviolet light exposure [9]. While beyond the scope of our current study, some common elements in plastics, notably Zn, are of concern due to toxic effects in biota, and marine life in particular [65,66,81].

Titanium, the most abundant element, is the common colorant in

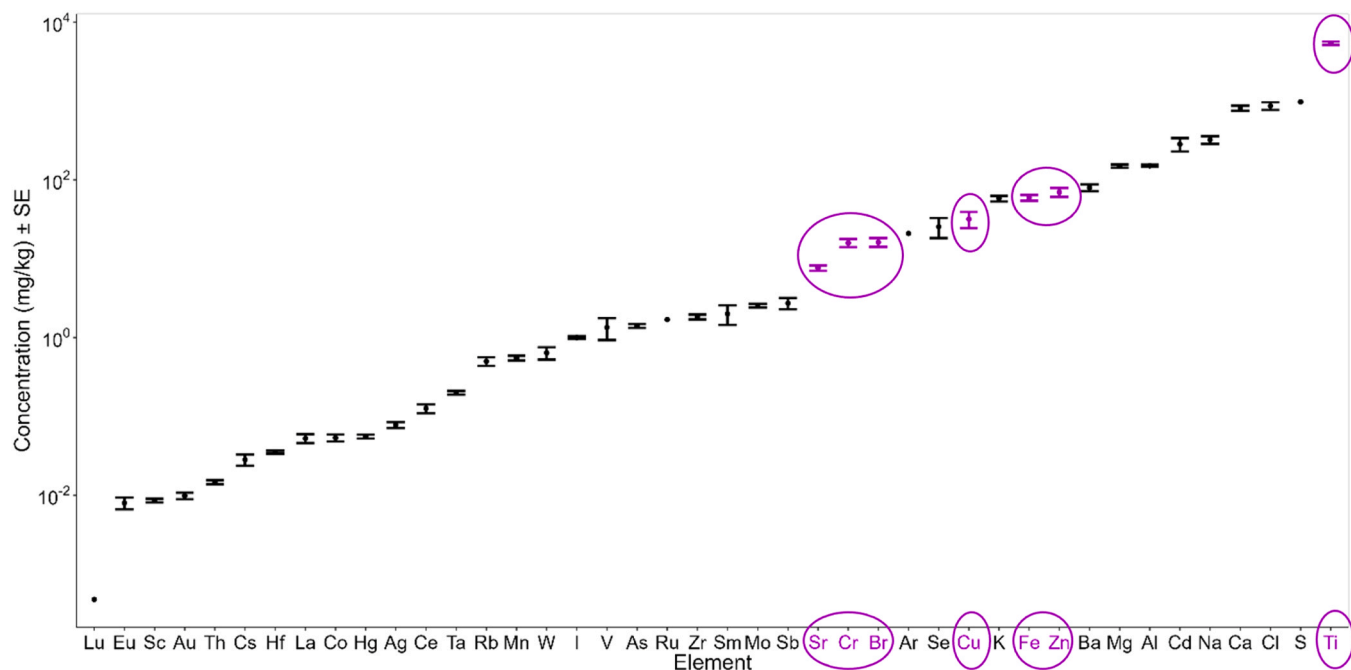
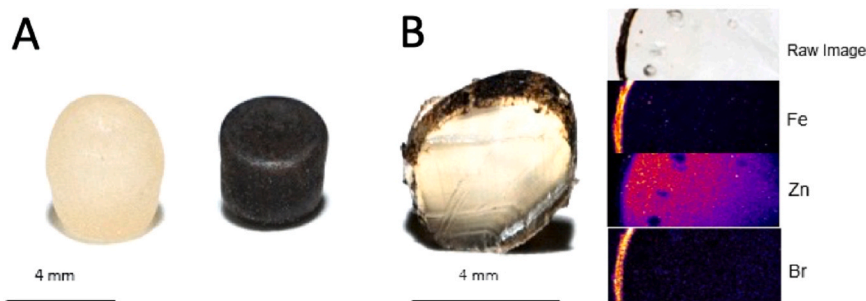
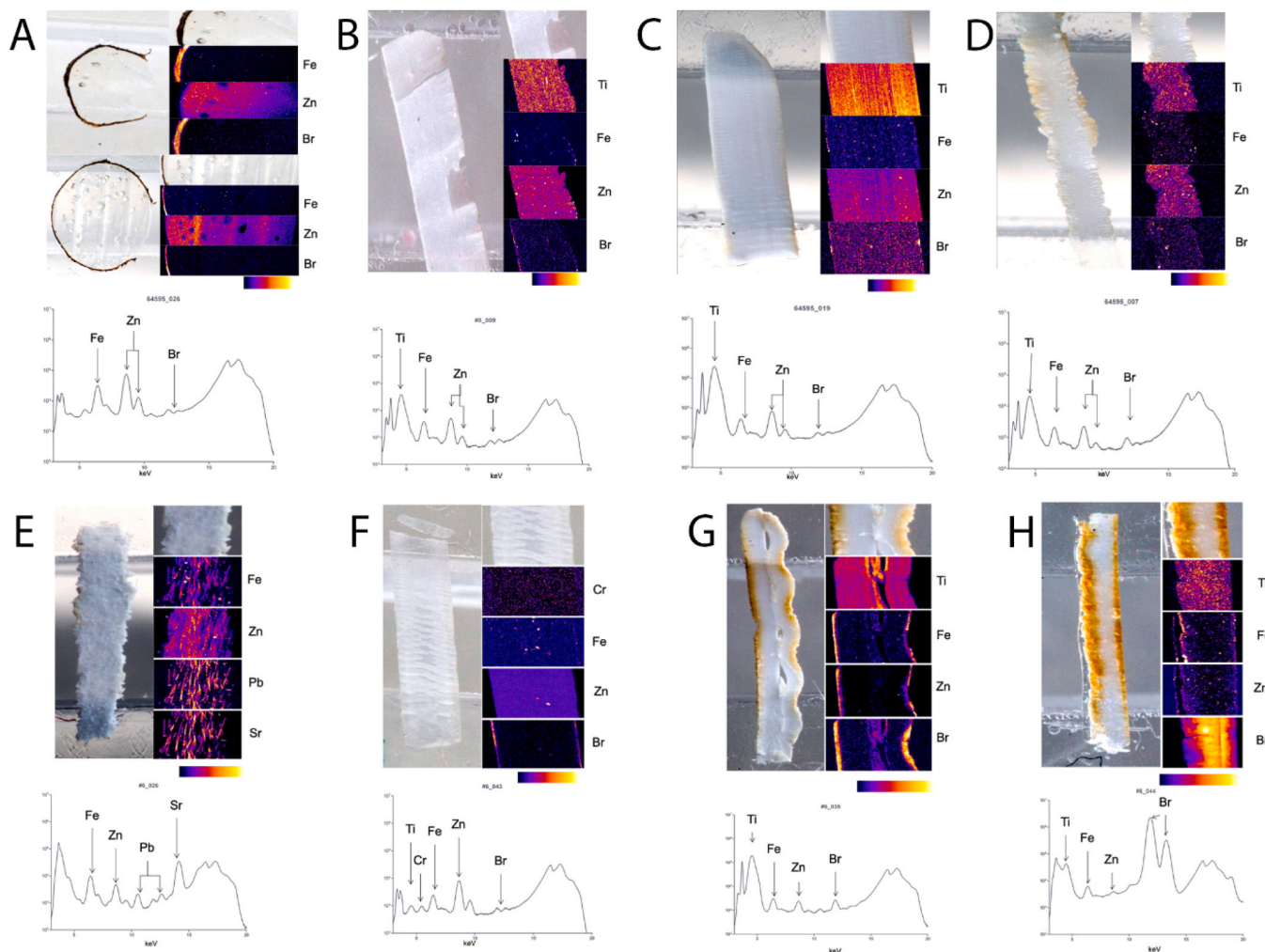


Fig. 2. Bulk measurements of the concentration of chemical elemental in the plastics retrieved from the stomachs of eight different shearwater fledglings. In the graph, the measured elements are sorted by increasing abundance. The within-fragment spatial distribution of the specifically high-lighted elements (Ti, Zn, Cu, Cr, Sr, Fe, Br – highlighted and circled in purple) was further studied in individual plastics fragments (Figs. 4 and 5). The elements Ti and Zn are present in most white plastics and are thus amongst the most abundant elements, while Cu and Cr are likely to be related to the colorants used in the manufacture of the coloured plastics fragments in the bulk samples. The presence of Br and Fe is most likely due to the accumulation of these elements as part of biofilm formation, as suggested by their prominent location at the surface of weathering plastics (Figs. 3–5). The presence of Sr hints at the presence of individual samples with Sr-containing additives.



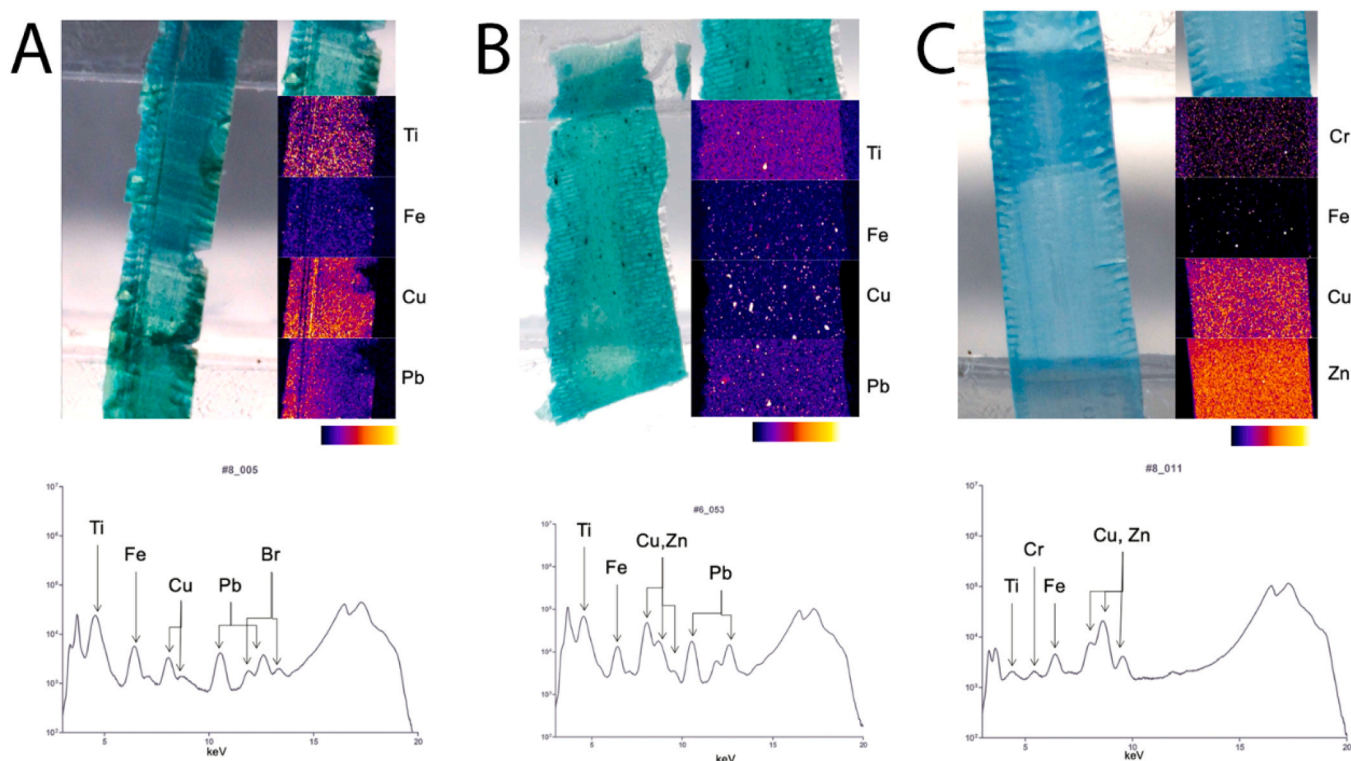
**Fig. 3.** (A) A virgin nurdle (unprocessed plastic pellet) and a weathered nurdle with the outer surface due to biofilm formation and deposition of elements. The black coloured pellet was retrieved from the stomach of an *A. carneipes* fledgling. (B) A cut through the weathered black nurdle revealed its original clear colour. Microtome sections (20 µm thick, 4 mm wide) mapped by X-ray fluorescence microscopy (9 µm, 16.5 keV beam) revealed internally the presence of Zn while the external surface contained iron (Fe) and bromine (Br).



**Fig. 4.** Synchrotron X-ray fluorescence microscopy (S-XFM) images of white plastics at different stages of weathering. The weathered unprocessed clear plastic nurdle (A) shows the presence of Zn throughout the entire plastic sample. Zn as a consistent additive was found in all investigated plastics. The weathered surface of the nurdle contained Fe and Br, a typical result of biofilm formation. All white plastics (B-H) contained titanium (Ti) with titanium oxide being a common white colorant and stabiliser additive - in slightly varying granularity, suggesting variations in the manufacturing process. The white fragment (E) from an unidentified plastics item contained prominent fibrillary structures that collocated with Pb and Sr as well as Fe. In addition to the typically present Zn and Ti in white plastics, a speckled distribution of Cr can be discerned through the body of this fragment (F). Advanced weathering of the external surface of the plastics fragments with clear surface accumulation of Fe and Br can be seen in the panel (G) and (H), a section through degrading white bottle cap. Beneath each of the optical and elemental images is the integrated x-ray spectrum from the measurement, which clearly indicates the major elements present in the specimen (see arrows). X-axis label is KeV.

white plastics, while Cu and Cr are related to the colorants used in the manufacture of the coloured plastics [13]. Our findings confirm previously reported elemental measurements in plastic packaging waste

product using NAA [61]. The presence of some elements with known toxicity [73], such as Pb and Cd, point to unregulated recycling [72] and use of polluted feedstock in manufacturing, though the epidemiology of



**Fig. 5.** In all green and blue coloured plastics fragments (A-C) synchrotron X-ray fluorescence microscopy (S-XFM) demonstrated the presence of Cu, albeit in varying densities throughout the volume of the material. The fragments shown in the image panels (A) and (B) additionally contained Pb, again in apparently different granularity, hinting at differences in the manufacturing process. The blue coloured sample shown in (C) potentially contains a small quantity of Cr in addition to Cu. Beneath each of the optical and elemental images is the integrated x-ray spectrum from the measurement, which clearly indicates the major elements present in the specimen (see arrows). X-axis label is KeV.

a multi-metal/mixtures and its impact, notably on vulnerable species is complex and remains to be explored [44].

The presence of Br and Fe was largely due to the prominent accumulation of these elements as part of biofilm formation, as suggested by their prominent location at the surface of weathering plastics (Figs. 3–5), though in some samples Fe was also found in the body of the fragment [55,62]. Several less abundant elements, such as lanthanides, gold, silver and others, found by NAA bulk analysis suggest that the origin of the ingested plastics may have been from recycled plastic [75]. The presence of Pb and Sr, too, hints at the presence of individual samples derived either from items with specialised function or are evidence of the materials' recycling history, notably regarding the Pb in plastics [74]. Since Sr was found throughout the matrix of some of the studied material (Fig. 4E) it is likely to be part of the originally manufactured plastics material rather than having been taken up from the environment. Strontium aluminate, for example, is an additive in 'glow-in-the-dark' paints and plastics while strontium salts have been used as stabilizers [80].

While the methodological approach in our study limits the number of samples that can be investigated, the data illustrate persuasively the heterogeneity in the elemental composition of plastics and the apparently universal presence of substantial surface changes of the fragments with enrichment of elements that are likely to reflect the presence of biofilm [35]. Importantly, the investigated material was retrieved from the stomachs of free-living wild seabirds and thus represents realistic exposure scenario.

The observed heterogeneity in the elemental composition of ingested plastics, notably recycled material, suggests that the theoretical toxicological risk for individual birds may vary greatly. Our data do not allow speculation about whether leaching of chemical elements or hazardous molecules from already weathered material remains a relevant health risk to wildlife. However, the observation that materials

decay (e.g., through oxidation or embrittlement; [27]) leads to the regular presence of biofilm growth and give grounds for speculation that the huge surface becoming available through fragmentation of plastics is highly likely to create a large, hitherto ignored ecological niche for microbial growth [4,79]. The extent and geographic, or context-dependent, emergence of biofilms associated with degrading plastics as an important part of the hazard mechanism found in marine waste plastic is now an active field of research [7].

The major impact of decaying plastics is akin to an ecosystem change at lower trophic levels at which the potential toxicity-increasing hazard mechanisms may be more severe than at higher trophic levels. The emergence of an additional ecological niche at lower trophic levels may also lead to potential bioaccumulation, biomagnification, or biofilm-mediated surface changes that may allow otherwise highly dilute pollutants or naturally occurring chemical elements, such as radioisotopes, to adsorb and accumulate at higher rate (e.g., [20,75]). Degrading plastics may thus become a potent vector for the entry of other potentially hazardous materials. The quantity of plastics in the marine environment is already thought to exceed 170 trillion particles (weighing 1.1–4.9 million tonnes; [21]) with predictions that the amount of ocean plastic will quadruple by 2050 [70]. Large microplastics (1.01–4.75 mm) typically account for > 40 % of all particles in the oceans [22]. If we assume a mean density of plastics of 0.95 g/cm<sup>3</sup> [48], approximate each piece as a sphere and use the mean mass per piece (0.013 g; [21]), we can estimate that the total surface area of ocean plastics to be 2000–10,000 km<sup>2</sup>, equivalent to approximately the area of Cyprus, Hawai'i (Big Island), or Bougainville Island, Papua New Guinea. This is a substantial potential surface area for biofilm colonization and the resulting accumulation of hydrophobic compounds from the ocean or from plastics intrinsically. The true value is in fact probably much higher given the pitted and uneven surface of weathered plastics.

Together with NAA, the detailed analysis by S-XFM illustrates the

dynamic nature of the weathering process, as well as an often not immediately recognisable compositional heterogeneity with the presence of toxic metals notably in individual weathered fragments of recycled plastics (Figs. 4 and 5). Future policies aimed at minimising potentially detrimental long-term effects of plastics waste need to proceed with the recognition that the establishment of dose-response relationships in regard to any inherent or acquired toxicity of plastics cannot be predicted without detailed understanding of the weathering patterns of decaying plastics, whereby an assessment of environmentally degraded, down-cycled, and reused plastics due to their nature as ‘composites of composites’ might not be feasible at all, and, therefore, these types of products need to be retained in a tightly closed loop of permanent custody (i.e., an exceptionally high level of Extended Producer Responsibility; [71]).

Presently, risk mitigation approaches focus on chemical toxicity which are relevant at the stage of production and early use of plastics. In the United States, the *Tox21* and *Toxcast* programs were developed to examine the toxicity of chemicals using high-throughput, rapid screening [56]. From 2007–2016, these programs generated toxicity data for ~9000 unique substances. However, with a new substance isolated or synthesized every 2.6 seconds, worldwide [1], the fate and toxicity of most chemicals remains unknown [68,77]. The regulatory backlog and forced prioritisation of a subset of chemicals, combined with the burden of proof required to demonstrate harm, flaunts the precautionary principle in a time of global environmental degradation [36], an approach that has been advocated for plastics for more than three decades [29,31].

The above-mentioned acceleration in the production and use of yet-to-be-assessed new chemical compounds [68,77], as well as our own observations, suggest that a reduction in the feed-stock variability that enters into current plastics products and reducing the decay rate of plastics might mitigate the cumulative risk. As an alternative to the development of more degradable plastics, the lowering of the net production and consumption of plastics and use of plastics materials with slower decay kinetics may provide a longer time window for reuse, recapture, storage and effective end-of-product life measures than uncontrolled release (as opposed to supervised composting, etc.) of highly (bio)degradable material where the net effect of creating an additional biological niche remains an unexplored hazard [45,78].

Finally, the observation of distinct elemental fingerprints that remain discernible even in advanced states of degradation suggests that purposefully added ratios of trace amounts of non-toxic, non-degradable chemical elements to plastics feedstock prior to or during different stages of manufacture into various goods can also be used to establish a chain of custody and quality control similar to hallmarking of precious materials. This approach has similarity to the addition of sequence-defined polymers for the purpose of creating materials traceability and thus the technical feasibility for Extended Producer Responsibility schemes for plastic waste [34]. Other approaches to enable traceability of plastics include the use of dyes, though both the permanence of the dye label as well as its potential toxicity upon leaching remain to be clarified [43,54].

The overall strategy to addressing the plastics waste challenge would then be avoidance of facultative use, and extension rather than reduction in a materials lifetime, combined with authentication and materially locked-in traceability (through addition decay resistant elemental or chemical signature) across their entire life cycle. Notwithstanding possible technical innovations and the normative ethics of environmental protection, the core of the current hyper-consumption crisis of plastics is a, possibly unique, mismatch between factual utility, price, true cost (including externalised costs) and perceived value. We, thus, point to a previous behavioural economics proposal to use elemental ‘fingerprinting’ or ‘hallmarking’ not only for the purpose of traceability but include also the addition of sufficient amounts of rarer elements (e. g., in the form of nano gold; [50,67]), that would incentivise the establishment of an unbroken chain of custody at the end of which might

stand the waste mining of the elements of value (equivalent to the externalised environmental or remediation costs) and the low emissions extraction of residual energy [69].

## Environmental implication

Plastics released into the environment enter complex decay pathways that include the release of toxic components, such as hazardous additives. Once ingested by wildlife, plastic-associated chemicals can be transferred to biota. Using spectral and neutron activation analysis, our ‘histological examination’ of plastics ingested by seabirds reveals the cumulative abundance of chemical elements that wildlife are commonly exposed to. Individual plastics of apparent macroscopic similarity were highly heterogeneous in the composition and distribution of chemical elements suggesting the internal spatial distribution of these elements will result in differential exposure during the weathering process.

## CRedit authorship contribution statement

**Puskar Ljiljana:** Writing – review & editing, Methodology, Formal analysis. **Banati Richard B.:** Writing – original draft, Supervision, Project administration, Investigation, Funding acquisition, Formal analysis, Conceptualization. **de Jonge Martin D.:** Writing – review & editing, Methodology, Formal analysis. **Bond Alexander L.:** Writing – original draft, Visualization. **Howard Daryl L.:** Writing – review & editing, Methodology, Formal analysis. **Lavers Jennifer L.:** Writing – original draft, Project administration, Investigation, Funding acquisition, Conceptualization. **Howell Nicholas R.:** Writing – original draft, Visualization, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at [doi:10.1016/j.jhazmat.2025.138528](https://doi.org/10.1016/j.jhazmat.2025.138528).

## Data availability

Data will be made available on request.

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