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Final report

AnalYsis of mlcroplastics and chEmicals in iNfant food (ALIEN)

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Abstract

The aim of this pilot study was to assess the presence and identify potential plastic packaging-associated chemicals and microplastic (MP) particles in two infant food products: one fruit-based and one dairy-based. MPs were found in both product types, with MP concentrations generally being higher across replicate samples of each product than in the procedural blanks. The results indicate that the detected particles originate primarily from the infant food products rather than from laboratory contamination. A range of polymer types were identified across samples, with particles identified as PE being the most detected across both products in almost equal amounts. The occurrence of PE is consistent with its use as the inner food-contact packaging material, suggesting that abrasion or degradation of the packaging may contribute to the MP content in the foodstuff. This is further supported by the observation that the estimated PE per gram of foodstuff is comparable across the two products. Given that PE is also one of the most widely used polymers globally, however, its presence may also reflect contributions from other points in the processing and manufacturing chain rather than the packaging itself. Furthermore, the spectral fingerprint of PE is very similar to that of lipids commonly present naturally in processed food items, and so its identification in this context should be considered as tentative. The presence of polyamide (PA), polypropylene (PP) and other polymers may also reflect contributions from other sources/points in the processing and manufacturing chain. Chemical analysis (Nontarget screening) revealed a higher number of tentatively identified chemicals in the plastic packaging than in either foodstuff, with 81 chemicals in the fruit puree and 111 chemicals in the yoghurt also being present in the respective packaging materials. A total of 53 chemicals in the fruit puree and 28 chemicals in the yoghurt were identified in the PlastChem database as being potentially plastic-associated compounds. However, the presence of these chemicals in the foodstuff does not necessarily reflect their migration from the packaging, as they may also have originated from other production steps. The results showed that MP and plastic-associated chemicals were present in both the fruit-based and dairy-based products tested, but targeted studies along the whole production-chain are needed to confirm identification and true origin to provide a robust basis for potential mitigation actions.



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1 Background and objectives

While recent research has documented the presence of (micro)plastic particles and plastic-associated chemicals in food and drink products for general human consumption, less focus has been given to the assessment of products specifically intended for consumption by infants. According to available studies, infant food products can be contaminated with a range of potentially harmful compounds, including inorganic chemicals, organic compounds, veterinary drug residues, pesticides, mycotoxins (e.g. Izzo et al., 2022), and microplastics (MPs) (Kadac-Czapska et al., 2022, Kadac-Czapska et al., 2023, 2024). Despite the potential human health implications, available information is very sparse and fragmented, preventing robust science-based conclusions from being drawn. Few studies have specifically focused on assessing food packaging as a source of MP contamination in products designed for infant consumption. Furthermore, while food contact materials (FCMs) are regulated and certain chemicals have been banned or heavily restricted (e.g. bisphenol A in the EU, Canada, China and USA), the human health implications of plastic-associated chemicals currently used in food contact materials (FCMs), as well as those from MPs, remain largely unknown.

Infant food in flexible multilayered pouches is a consumer market estimated to grow annually (e.g. ~5% between 2024-2028 according to Technavio, 2024). Squeezable food packaging materials are generally made of a three-layer lamination consisting of an outer layer (typically of PET), a central functional barrier (typically of PET/Aluminium foil/PE), and an inner layer (typically PE). The outer layer is reverse printed in eight to ten colours and heat-sealed to the film. Aluminium foil is used as a functional barrier between the colourants/prints and the food contained within. As aluminium is acidic and salt-soluble, the inside surface of squeezable pouches in direct contact with the food has an inner layer of PE to prevent the migration of aluminium ions to the foodstuff (Bauer et al 2019). Such infant food packaging products are also typically equipped with a spout and cap, in most of the cases made of high density PE (HDPE).

Multiple factors can influence the migration of plastic additive chemicals, printing inks and non-intentionally added substances (NIAS; e.g. monomers) from packaging materials into food products. Key among these are the composition of the packaging material, the type of polymer used, the nature of the food matrix, and the physicochemical properties of the additives/NIAS incorporated within the polymer matrix. Food-related parameters such as lipid content, moisture level, and pH can strongly affect the rate and extent of additive migration (Gupta et al., 2024). In addition to chemical migration, MP particle formation and contamination may also occur, either through the degradation or mechanical abrasion of packaging materials or by entering during the food production, processing and handling processes. Importantly, the potential sources of MP and chemical contamination are not limited to packaging materials, as they may also arise from the wider production and supply chain, including processing equipment, transport, and storage. Identifying and attributing the specific origin of MP and chemical contaminants can, therefore, be challenging, particularly when the packaging is composed of common thermoplastics such as PE and PET, which are polymers widely used across multiple stages of food production and which are also very common polymers in many consumer products with different origins (Giri et al., 2024).

Greenpeace International (GP) commissioned SINTEF Ocean (SO) to conduct a pilot project with the combined aims of:

- (i) Quantifying and characterising the MP (20 µm-5 mm) content in fruit-based (fruit puree with apple, blueberries and oats) and dairy-based (yoghurt) pouch products designed for infant



- consumption to determine the proportion of MP that may derive from the plastic packaging materials directly in contact with the foodstuff.
- (ii) Assessing the potential migration of plastic-associated chemicals from the plastic packaging materials into the foodstuffs using analytical chemical screening.

These aims were achieved through the following research objectives:

Microplastic

- Generate Raman spectra from the sample packaging to be used as a reference for the MP screening.
- Verify that the selected food sample digestion steps have a negligible impact on the reference package material (i.e. fragmentation that leads to over estimation of the number of MP particles).
- Apply a validated digestion method to remove biological material (i.e. the food matrix) and facilitate high quality polymer identification and quantification.
- Characterise the physicochemical properties of the isolated MP (polymer composition and size) using a combined microscopy and μ Raman analysis approach.
- Quantify the *number* of MP particles in the foodstuff samples using microscopy and μ Raman analyses.

Plastic-associated chemical screening

- Determine the effectiveness of extraction and cleanup methods for isolating plastic-associated chemicals from complex food matrixes.
- Identify the potentially plastic-associated chemicals (e.g., phthalates, BPA, antioxidants, UV stabilizers) in infant food packaging and the foodstuff using a non-target screening (NTS) approach with comprehensive two-dimensional gas chromatography mass spectrometry (GCxGC-MS) instrumentation.
- Generate a list of identified chemicals present in the plastic packaging
- Generate a list of identified chemicals present in the foodstuff • Compare additive presence in the packaging and foodstuff matrices.

2 Material and Methods

2.1 Microplastics analyses

2.1.1 Validation of extraction procedure and reference particles

Reference microparticles (RMP) from the packaging of both infant food products provided by Greenpeace were artificially produced in the laboratory. The packaging samples were cut as small as possible with scissors to produce the RMPs (ca. between 1000-2000 μ m). Eleven randomly selected RMPs from different areas of the fruit pouches were individually morphometrically and spectroscopically characterised by shape, size and colour using μ Raman automated imaging and spectroscopic analysis (Soleil, Horiba, Japan) and the associated instrumental software (LabSpec 6.8.1). Similarly, for the dairy pouches, 11 RMPs were selected and evaluated. Analyses were performed using a 785 nm excitation laser and a 300 grating. The laser intensity was set with a 20% neutral density (ND) filter applied. The acquisition time was 0.4 seconds with 50 accumulations per spectrum. In addition to the RMP from the pouches, part of the cap in contact with the food was also spectroscopically characterised to confirm the polymeric composition. The RMP physicochemical characterisation was performed on both sides of each particle to ensure the internal layer in contact with the foodstuff and the external layer corresponding to the outside part of the pouch could be



distinguished. After the pre-digestion characterisation step, 11 RMP from the fruit product pouch and 11 RMP from the yoghurt pouch were exposed to the digestion treatment selected to separate and extract the MP from the foodstuff matrix to assess the potential impacts of the digestion process on the RMP physicochemical properties. The RMP were sequentially suspended in 10% potassium hydroxide (KOH) solution and 30% hydrogen peroxide (H_2O_2). The RMP remained in the KOH solution for 72 hours and in the H_2O_2 solution for 24 hours, which represents the approximate time needed for a successful digestion of the real foodstuff sample (see Section 2.1.2). After this time, a post-digestion morphometric and spectroscopic characterisation of the RMP was performed according to the same pre-digestion procedure described above. The physicochemical characterisation and comparison of the pre- and post-digestion treatment of the RMPs allowed any changes to the RMP physicochemical properties arising from the digestion procedure to be identified.

2.1.2 Extraction and characterisation of MP from the foodstuff

A foodstuff sample (approximately 10 g wet weight) was taken from each pouch (n=3 samples for both products) and subjected to the MP extraction, quantification and characterisation protocol. In addition, processing/laboratory blanks were prepared following the same procedure, but without the use of any foodstuff. These blank samples (n=3) were run alongside the foodstuff samples to account for laboratory contamination (see Section 2.1.3). Each subsample was weighed into a 100 mL pre-baked and milli-Q rinsed glass beaker and exposed to 50 mL of pre-filtered 10% KOH at 50 °C for 72 hours. After the KOH exposure, the digestate was fractionated on a 300 μ m Nylon filter (diameter 4.5 cm, PLASTOK, UK) and a 10 μ m stainless steel filter (Teichhansel, Germany) to facilitate up concentration of the sample. The material retained on the two filters was rinsed off with 30 % H_2O_2 (50 mL) into a clean 100 mL glass beaker and left to digest for 24 hours at 50 °C. After the H_2O_2 exposure, each digestate was fractionated once again on the two filters, as described above. The fraction >300 μ m (MP_{Large}) was retained on the filter for direct microscopic inspection. The smaller fraction (20-300 μ m) was sonicated (50 seconds) and re-suspended in a 50% ethanol solution to both remove the particles from the filter and dissolve any remaining biogenic molecules before further processing and analysis.

MP_{Large} : The material >300 μ m retained on each filter was visually inspected under a stereomicroscope (SMZ745T Nikon). Particles and fibres were manipulated with stainless steel tweezers during the identification process to help exclude non-plastic particles from the sample. Particles/fibres exhibiting an obvious cellular/natural structure or that were clearly part of the foodstuff were excluded as organic material. No particles were identified as potentially being plastic in this fraction for both the fruit and dairy products, and therefore no further analyses were performed for this size fraction.

MP_{Small} : The 50% ethanol suspension was homogenised and a 1 mL subsample filtered through a 5 μ m pore size silicon filter (Smart membranes, Germany). Although a relatively small sample volume was used, the suspension still contained a substantial number of undigested particles. Limiting the amount of material on the filter is essential to avoid overloading and to ensure optimal μ Raman measurements. Raman analyses were performed using a 532 nm excitation laser and a 600 grating. The laser intensity was set between 95–100%, with a 20% neutral density (ND) filter applied. The acquisition time was 0.3 seconds with 30 accumulations per spectrum. MP were identified from mosaic images using LabSpec6 software with the associated reference spectral libraries. A Hit Quality Index (HQI) threshold of $\geq 80\%$ was applied for spectral matching. As both the inner surface of the packaging and the food-contact area of the cap were identified as polyethylene (PE) (see Results section), all spectra initially assigned to a polymer type were manually



reviewed to ensure the correct identification (see the Results section for a discussion about the uncertainty about PE identification). MP measured by Raman spectroscopy are reported as the number of MP per mL of digestate sample, and should not be confused with the estimated number of MP per gram of food. The quantification of total MP in each sample is presented as the average number of MP \pm standard error (\pm SE), while the polymer and size composition data are presented as the actual number of MP for each analysed subsample. Statistical analyses were performed on the measured quantities of MP. As the data did not meet the requirements for normality and homogeneity required for parametric statistics, the differences in MP total quantities, polymer and size composition were separately assessed using PERMANOVA (PRIMER v.7):

- (i) foodstuff samples vs procedural blanks
- (ii) fruit puree vs yoghurt

Assessment was based on Euclidean distances with 9,999 unrestricted permutations of residuals under a reduced model and a significance level of 5%.

2.1.3 Anti-contamination procedures

Special attention was given to limiting sample contamination by airborne MP, with precautions implemented at every step of sample processing by following the anti-contamination protocol described in Piarulli et al. (2019). Briefly, MP extraction was performed in a clean laboratory where all surfaces were pre-cleaned with acidified Milli-Q water prior to processing the samples. Plastic equipment was entirely replaced with metal and glass alternatives wherever possible, which were rinsed with Milli-Q water before use. Contact with air and plastic surfaces during all laboratory procedures was minimised for samples, instruments and reagents by covering them with Milli-Q rinsed aluminium foil before and after use. After filtration, filters were kept in covered glass petri dishes that had previously been rinsed with Milli-Q water. All solutions and Milli-Q water were pre-filtered on 10 μ m glass microfibre filters (Whatman®, UK). The use of cotton clothes and lab coats was mandatory to access the clean laboratory. To validate the effectiveness of the contamination prevention approach, 3 procedural blanks (sample-free digestion solutions) were treated identically to the foodstuff samples. Material retained on the filters from the procedural blank samples was carefully examined following the same procedure as for the foodstuff samples (see Section 2.1.2) to identify any external MP contamination that should be accounted for.

2.2 Chemical screening

2.2.1 Preparation of the materials.

The content of the fruit and dairy infant pouches was transferred into pre-baked glass bottles and subsequently freeze-dried. Prior to extraction, 2 g of the freeze-dried food was weighed into glass vials. The empty plastic pouch was then rinsed with Milli-Q water to remove any residual foodstuff prior to extraction and analysis of the packaging material. Three procedural blanks were extracted alongside each type of sample.

2.2.2 Solvent extraction

Triplicate samples of the interior surface (food contact zones of the material) of each plastic pouch were individually extracted by adding ethyl acetate (EtAc; 10 mL) and ultrasonication for 30 min at 60 °C. The EtAc was then transferred to a glass beaker and a secondary extraction with dichloromethane (DCM; 10 mL) was conducted with ultrasonication for 30 min at room temperature. It is important to highlight that the extraction of the pouch material itself was performed by adding the solvent directly into the pouch. The EtAc and DCM extracts were then combined, filtered (0.7 μ m glass fibre) to remove any particulate material



that may have transferred from the pouch, and volume adjusted to approximately 1.5 mL by gentle evaporation with nitrogen gas and transferred to 2 mL glass vials. Three lab blanks were extracted by adding the solvents into prebaked vials. The same procedure (EtAc and DCM with ultrasonication) was applied for the extraction of the freeze-dried food samples. In this case, the extraction solvents were added directly into the individual glass vials containing the 2 g samples. In addition, 3 samples of prebaked sodium sulphate (Na_2SO_4) were extracted alongside the samples as procedural blanks to account for contamination during sample processing and analysis.

2.2.2 GCxGC-MS analysis

Chemical analysis was performed using a 7890B gas chromatograph coupled with a 7250 quadrupole time of flight mass spectrometer and interfaced with a Zoex ZX2 cryogenic modulator. The first-dimension column was a Zebtron ZB-1ms (30 m × 0.25 mm × 0.25 μm) and the second-dimension column was a BPX50 (1.0 m × 0.25 mm × 0.25 μm). The two columns were interfaced with a 1 m × 0.25 mm deactivated fused silica modulation loop. The carrier gas was high purity helium at constant flow (1.1 mL/min). Samples (1 μL) were injected at 250 °C splitless. The oven temperature was kept at 60 °C (1 min hold), ramped by 5 °C/min to 300 °C (10 min hold). The hot jet was offset at 70 °C (1 min hold), ramped by 7 °C/min to 360 °C (10 min hold). The modulation time was 6 s with a 350 ms pulse length. The transfer line temperature was 300 °C, the ion source temperature was 200 °C, and the quadrupole temperature 150 °C. The EI source was operated at 70 eV. Scan speed was 50 Hz, and the recorded mass range 50-650 m/z.

2.2.3. Data treatment

MassHunter Unknowns Analysis software (version 10.0) was applied to the raw data files for deconvolution and tentative identification of analytes using a query towards the NIST23 mass spectral library, returning up to five matches with a similarity of >80 % for each analyte. In cases where more than one match >80% was returned, the candidate chemical with highest match was selected. Output files containing all peaks and their tentatively assigned identities were then exported to .csv format for further processing using R studio (version 4.5.0, R core Team). To harmonize the retention times (RT) of the same analytes across the different samples, the first- and second-dimension RTs were calculated relative to a defined modulation period and baseline peak. Compounds were grouped if they occurred within a (0.2-minute first dimension, 0.2 second dimension) RT window and shared a common mass spectral identifier, thereby accounting for minor shifts in peak position that can occur when analysing multiple samples. To reduce background interference, any analytes detected in blank samples were excluded from the corresponding food and packaging datasets. In addition, duplicate hits within the same sample were merged by averaging the peak areas. Finally, analytes that were found in both the package and the foodstuff were compared to identify the overlapping compounds. The chemicals tentatively identified in both the plastic package and in the foodstuff were cross referenced with the PlastChem database ([Monclús et al. 2025](#)) which is one of the most updated databases allowing for the identification of the plastic related chemicals and their use (see results section). This database compiles existing information on the hazards, functions, uses, occurrence, production volumes, and regulatory status of chemicals used in or present within plastics. It is important to note that many of these chemicals also have other applications and are not unique to plastics.



3 Results and discussion

3.1 Microplastic analyses

3.1.1 Validation of the extraction procedure and reference particles

After exposure to the sequential digestion procedure with KOH and H₂O₂ over a period of approximately 96 hours, the RMPs (n=11 from the fruit puree packaging and n=11 from the yoghurt packaging) did not show significant alteration in their physical properties (Figure 1). The average (\pm SE) size of the RMP from the fruit puree packaging before the digestion procedure was 1804 (\pm 31) μ m (maximum Feret diameter) and 1239 (\pm 59) μ m (minimum Feret diameter), while it was 1794 (\pm 46) (maximum Feret diameter) and 1241 (\pm 77) μ m (minimum Feret diameter) after the digestion procedure. The average (\pm SE) size of the RMP from the yoghurt packaging before the digestion procedure was 1102 (\pm 85) μ m (maximum Feret diameter) and 667 (\pm 55) μ m (minimum Feret diameter), and 1021 (\pm 61) (maximum Feret diameter) and 627 (\pm 44) μ m (minimum Feret diameter) after the digestion procedure. Furthermore, sharp edges and corners on individual RMPs from both types of packaging were retained after the digestion process. A few particles exhibited partial delamination of the inner layer from the outermost layers. This effect is most likely attributable to the particle production process rather than to the digestion treatment itself. Therefore, this effect was considered negligible in the context of this project.

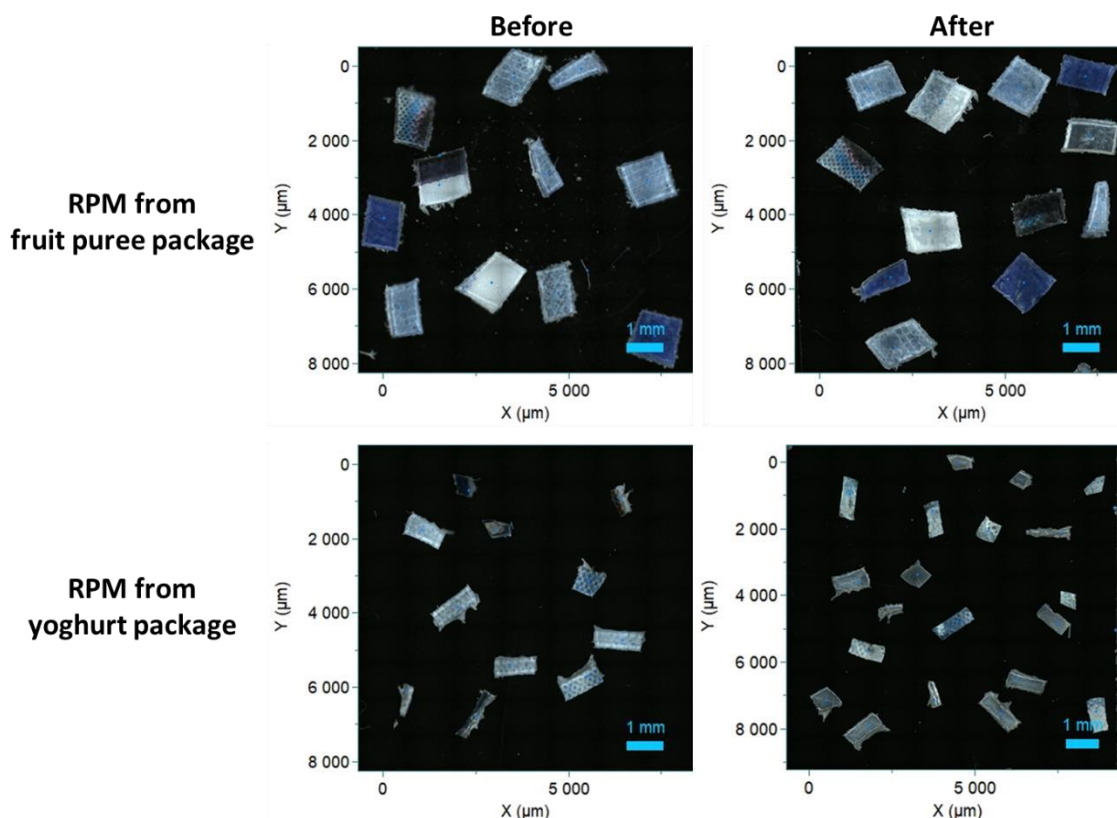


Figure 1: Photographic examples of the RMP from the packaging (internal layer of the pouch in contact with the foodstuff) of the two tested products before and after the sequential exposure to KOH and H₂O₂ digestion treatments.



The internal layer of the RMPs for both products was spectroscopically confirmed as PE both before and after the digestion process, suggesting no chemical alteration of the fruit packaging RMPs (Figure 2A, B, D) nor the yoghurt packaging RMPs (Figure 3A, B, D) had occurred as a result of the digestion treatment. The polymer composition of the cap in contact with the foodstuff was also confirmed as PE for both products (Figures 2C and 3C).

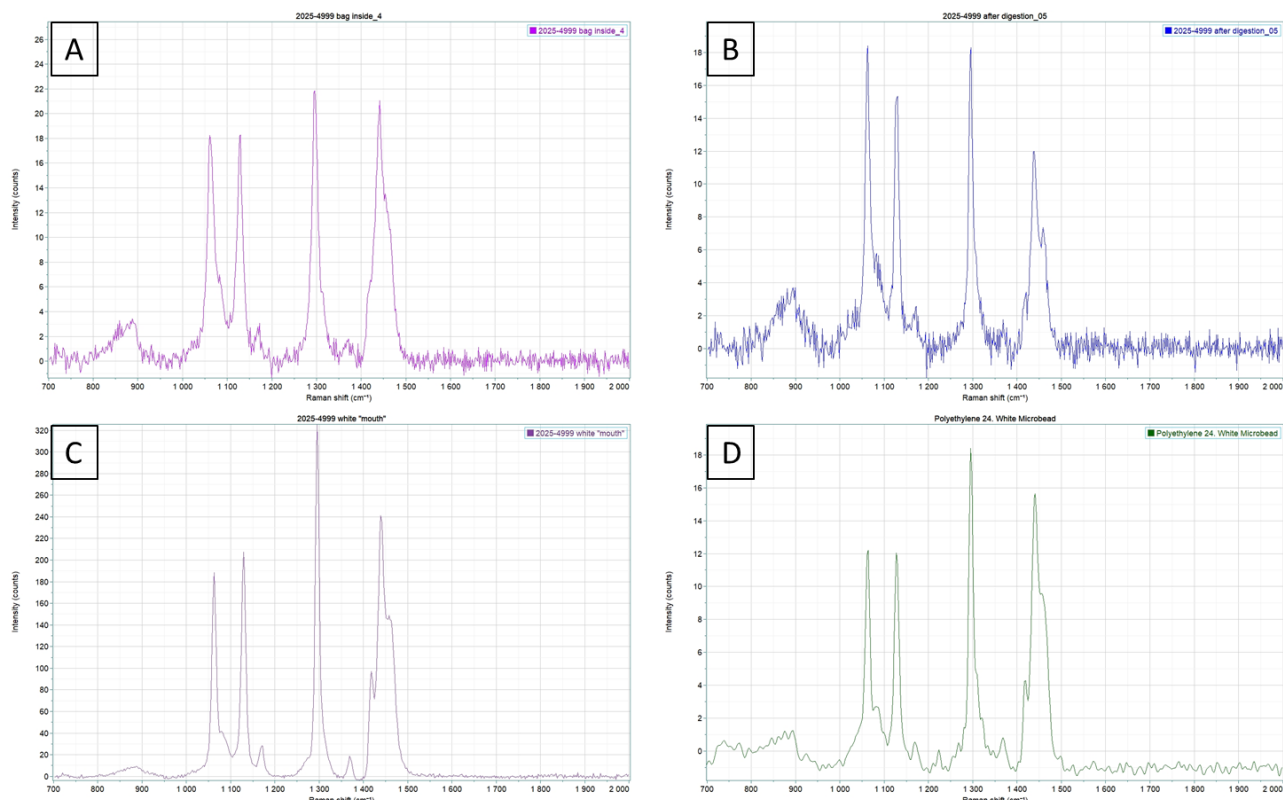


Figure 2: Example of Raman spectra of the RMP from the fruit puree packaging before (A) and after (B) the digestion treatment, the part of the cap in contact with the foodstuff (C), and the PE reference spectrum from the library (D).

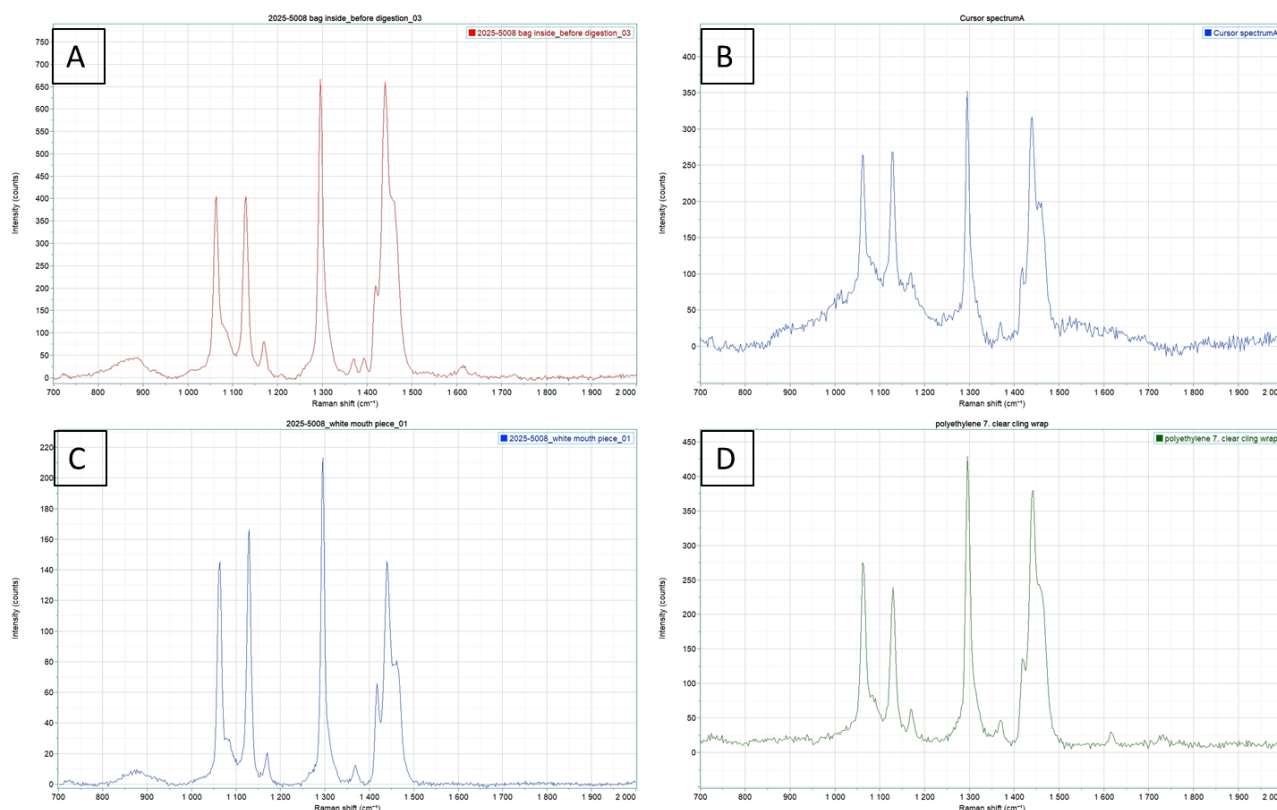


Figure 3: Example of Raman spectra of the RMP from the yoghurt packaging before (A) and after (B) the digestion treatment, the part of the cap in contact with the foodstuff (C), and the PE reference spectrum from the library (D).

3.1.2 MP in the foodstuff samples

MP analyses for the MP_{small} fraction (20–300 μm) showed that both the fruit and yogurt food products contained significantly higher MP concentrations (13.5 ± 2.6 MP mL⁻¹) than the procedural blanks (3 ± 1 MP mL⁻¹) (Figure 4; PERMANOVA, $p = 0.006$). These total MP numbers include particles that were confirmed as MP and those that are tentatively identified as MP (see discussion about the uncertainty below in this paragraph). Polymer composition also differed significantly between food samples and blanks (PERMANOVA, $p = 0.04$), indicating minimal background contamination during sample processing (Figure 5). Blank samples contained fewer polymer types and lower MP quantities overall, with only small amounts of common polymers (e.g., PE, PA, PP, and PBT depending on the associated matrix). Overall, these results show that MPs detected in both the fruit and yogurt foodstuffs are primarily associated with the food products rather than laboratory contamination.

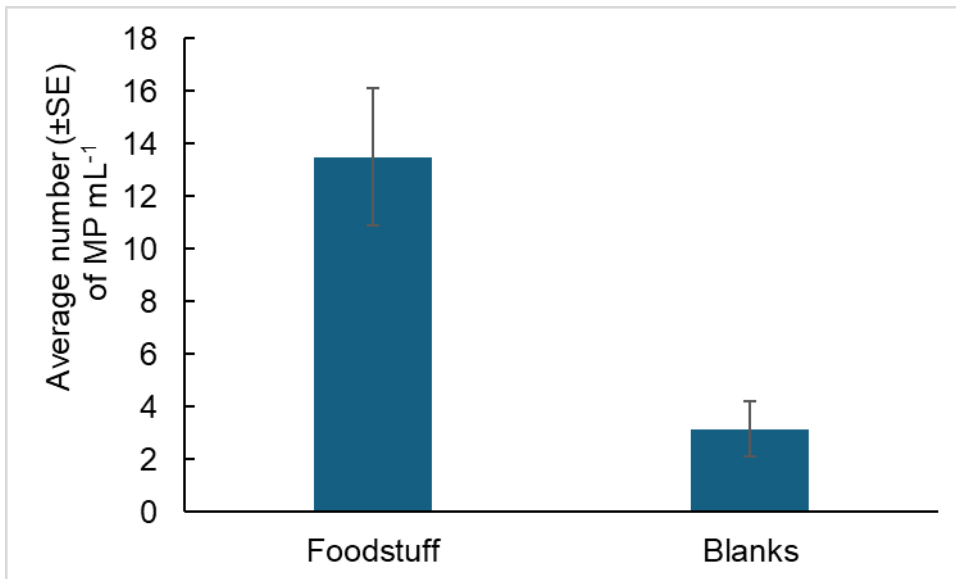


Figure 4: Average number (\pm SE) of identified MP mL⁻¹ in the digestate of the foodstuff (both fruit and yoghurt) and in the associated procedural blanks.

When comparing the two different food matrices with each other, the fruit-based product was found to contain slightly higher MP concentrations (18 ± 3 MP mL⁻¹) than the yoghurt-based product (9 ± 1.6 MP mL⁻¹), although the difference was not statistically significant (PERMANOVA, $p > 0.05$). Polymer composition also did not differ significantly between the matrices (PERMANOVA, $p = 0.1$). Fruit samples exhibited a broader polymer variety, with polyethylene (PE) and polyamide (PA) particularly abundant in replicate #3, with additional contributions from polypropylene (PP), polystyrene (PS), ethylene–vinyl acetate (EVA), and others (Figure 5). The yoghurt samples were dominated by PE and PP, with smaller proportions of PA and PS. Additionally, no clear matrix-specific trends were observed in MP size distribution. Across all sample types, the majority of particles (43–100%) were 20–50 μ m, followed by 50–110 μ m (4–57%), with only a small fraction in the 110–300 μ m range (4–8% in the fruit product) (Table A1, Appendix 1).

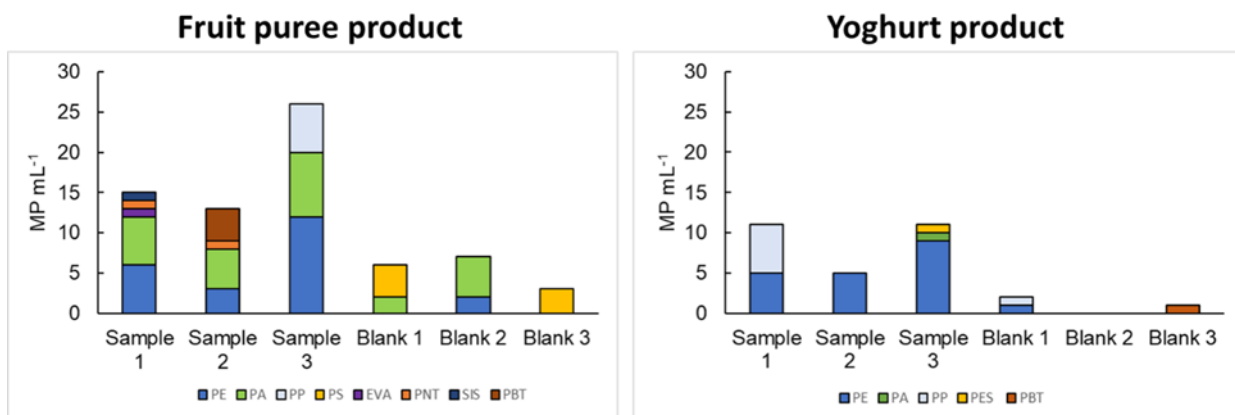


Figure 5: Number and polymer composition of MP mL⁻¹ of analysed replicated digestate subsamples (1 mL from each replicated sample). PE=polyethylene; PA=polyamide; PP=polypropylene; PES=polyester; PS=polystyrene; EVA=ethylene vinyl acetate; PNT=polynepentylene terephthalate; SIS=isoprene-based copolymer; PBT=polybutylene terephthalate.



By extrapolating the MP concentrations measured in the analysed 1 mL subsamples to the total mass of the foodstuff samples (10 g from each pouch) from both products, the number of total MP and PE per gram of foodstuff and for the entire pouch can be estimated (Table 1). Interestingly, the estimated mass of PE g^{-1} of foodstuff was very similar between the two foodstuff matrices. This corresponded to an average total MP abundance of $99 \pm 12 \text{ MP g}^{-1}$ in the fruit puree and 54 ± 10 in the yoghurt, of which 37 ± 9 and 38 ± 7 were PE MP g^{-1} , respectively. Although these extrapolated values offer only an approximate indication of MP levels, and should be interpreted with caution, they suggest that the number of PE particles is comparable across both food types. Notably, PE is the primary polymer used in the inner food-contact layer of the packaging. Its presence in both matrices at comparable levels is, therefore, consistent with the hypothesis that abrasion or fragmentation of the packaging during processing, storage, or handling may act as a source of MP contamination in the foodstuff. However, PE also represents approximately one-third of global plastic production (Plastics Europe, 2020), meaning that other potential sources of PE within the food production chain cannot be excluded. Furthermore, the internal PE layer of the pouch appeared white/transparent and did not present distinctive spectroscopic features that may allow differentiation between PE originating from the packaging and PE potentially introduced from other sources. This consideration applies similarly to the other polymers detected. As they do not form part of the packaging material and their negligible presence in the blank samples means they are unlikely to originate from laboratory handling or analytical procedures, it is most likely that they derive from equipment, processing or other materials used during manufacturing process. The only polymer that may indicate laboratory contamination is PA, which exhibits similar levels both in the fruit puree and two of the associated procedural blanks, but was not observed in the procedural blanks of the yoghurt.

Table 1: Estimated average values (\pm SE) of MP and PE per gram of foodstuff product and estimated MP and PE per pouch. Columns marked with asterisks (**) indicate that the values for the two products are not directly comparable because the fruit puree pouch contains a nominal weight of 113 g of foodstuff, whereas the yoghurt pouch contains 99 g. It should also be noted that PE should be considered as tentatively identified.

Product	Estimated total MP g^{-1} of foodstuff	Estimated PE g^{-1} of foodstuff	Estimated total MP pouch-1 **	Estimated PE pouch-1 **
Fruit puree	99 (\pm 12)	37 (\pm 9)	11187 (\pm 1316)	4215 (\pm 1050)
Yoghurt	54 (\pm 10)	38 (\pm 7)	5346 (\pm 970)	3762 (\pm 647)

While manual inspection and quality assurance of the Raman spectral matches was performed, it is important to note that PE spectra are known to be essentially identical to the spectra of lipids, particularly long-chain fatty acids such as stearic acid (Lim and Shin, 2025), which are abundant in (processed) vegetable and (both processed and unprocessed) dairy food matrices (Elmadfa and Majchrzak, 2000). This spectral similarity can complicate polymer identification and may lead to tentative or uncertain assignments (Araujo et al., 2018). The 50% ethanol rinsing step employed in the current study should have removed such molecules from the sample prior to Raman analysis, however, given the complexity of the matrix, complete removal cannot be guaranteed particularly in the absence of foodstuff samples that have not been exposed at any stage of the production chain to potential MP contamination. Therefore, the identification of PE in this context should be interpreted cautiously and regarded as putative. In addition to the spectral uncertainties associated with PE, it is important to acknowledge that Raman spectroscopy may also face challenges in reliably distinguishing PA from protein-rich matrices. This overlap in spectral features may represent an additional source of uncertainty in polymer identification. The fruit product, where PA was mainly identified, is not expected to contain substantial amounts of proteins suggesting PA is a more likely



identification. Based on the nutritional information on the packaging, this particular product consists primarily of carbohydrates, sugars, and fibres. Therefore, the possibility of PA spectral misinterpretation is considered limited in the context of this project.

3.1 Chemical screening

3.1.1 Tentative identification of chemicals

Fruit puree product

Both the fruit foodstuff and pouch packaging sample types were found to contain a high number of total detectable chemical features (automatically deconvoluted peaks, no identity assigned), with the plastic packaging extracts exhibiting a higher average number of chemical features (8591) than the fruit extracts (6853). Across replicates, a total of 1029 different chemical features (out of 8591) could be tentatively identified in the plastic extract based on their spectral similarity to library compounds (percentage match to NIST23 spectra >80 %) (Table A2). Owing to the non-target screening approach used for these analyses, the identification of the compounds is considered to be tentative unless standards are used for confirmation. For the fruit extracts, a total of 856 chemical features were tentatively identified across the replicate samples (Table A3). After RTalignment within the dataset, exclusion of background chemicals, and consolidation of duplicate chemical identifiers, the replicate plastic pouch extracts were found to contain an average of 394 tentatively identified compounds, with the replicate fruit extracts containing an average of 300 tentatively identified compounds. A total of 83 tentatively identified compounds were found in both the packaging and fruit samples (Figure 6). These compounds were further examined to assess their relevance in plastic materials generally. Cross referencing with the PlastChem database, an inventory of chemicals known to be used in or associated with plastics, revealed that 55 of the 83 common chemicals to the packaging and fruit are potentially plastic related (Table 2). However, it is important to note that the presence of these compounds in both samples does not necessarily confirm that they have leached from the packaging material to the foodstuff. Many of the tentatively identified chemicals have multiple industrial and commercial uses, including applications as fragrances, stabilizers, or biocides. Their detection may therefore reflect broader environmental or product-related sources rather than direct migration from packaging. Furthermore, the presence of these chemicals in the food material and subsequent adsorption to the inner surface of the plastic pouch packaging material may also have occurred.

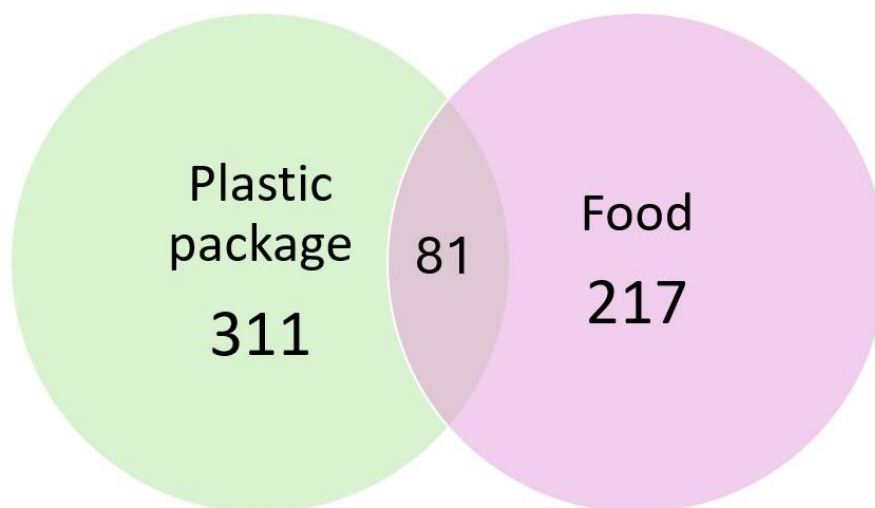


Figure 6: VENN diagram showing number of tentatively identified chemical features in the plastic packaging extracts, in the fruit foodstuff, and those common to both matrices.

Table 2: List of 81 chemicals tentatively identified both in the plastic package and in the foodstuff. The compounds marked as orange are those that are known to be used in or have been found in plastics according to the PlastChem database (Monclús et al. 2025), while those marked in grey are those not present in the database. NA = not applicable

CAS number	Name	Identified as plastic chemical	Use
1000336-54-1*	Butyl 9,12-octadecadienoate		NA
1000357-25-8*	1, 1, 5-Trimethyl-1, 2-dihydronaphthalene		NA
1000405-19-1*	trans-9-Octadecenoic acid, pentyl ester		NA
1000406-32-3*	Triacontane, 1-iodo-		NA
1000406-32-4*	Dotriacontane, 1-iodo-		NA
1002-84-2	Pentadecanoic acid		Lubricant; other processing aids
10032-15-2	Butanoic acid, 2-methyl-, hexyl ester		Not specified
10191-41-0*	dl-.alpha.-Tocopherol		Antioxidant; colorant; filler; light stabilizer; odour agent; other processing aids
112-12-9	2-Undecanone		Not specified
112-40-3	Dodecane		Lubricant



112-62-9	9-Octadecenoic acid (Z)-, methyl ester		Lubricant
112-79-8	9-Octadecenoic acid, (E)-		Not specified
112-80-1	Oleic Acid		Colorant; crosslinking agent; Filler; heat stabilizer; intermediate; lubricant; monomer; odour agent; other processing aids; plasticizer
112-92-5	1-Octadecanol		Biocide; colorant; filler; intermediate; lubricant; odor agent; other processing aids; plasticizer
120-95-6	Phenol, 2,4-bis(1,1dimethylpropyl)-		Intermediate
121-33-5	Vanillin		Biocide; lubricant; odour agent; other processing aids, flavouring agent
122-99-6	Ethanol, 2-phenoxy-		Antistatic agent; biocide; colorant; filler; intermediate; light stabilizer; lubricant; odour agent; other processing aids; plasticizer
124-07-2	Octanoic acid		Biocide; colorant; filler; intermediate; lubricant; monomer; odour agent; other processing aids; plasticizer
125456-63-5	(2E,6E,10E)-3,7,11,15-Tetramethylhexadeca-2,6,10,14tetraen-1-yl formate		NA
13038-47-6	9,11-Octadecadienoic acid, methyl ester, (E,E)-		NA
13474-59-4	trans-.alpha.-Bergamotene		Essential oils from plants
148-03-8	.beta.-Tocopherol		
1560-98-1	Octacosane, 2-methyl-		Not specified
18252-46-5	cis-.alpha.-Bergamotene		Essential oils from plants
18435-45-5	1-Nonadecene		Not specified
18835-32-0	1-Tricosene		Not specified
18835-35-3	Nonacos-1-ene		NA
20170-32-5	3,5-di-tert-Butyl-4hydroxyphenylpropionic acid		Antioxidant; light stabilizer; lubricant
21145-77-7	Tonalid		Fragrance
2117-34-2	Silane, triethylmethoxy-		NA
2277-16-9	4-Nonenal, (E)-		Not specified



2363-88-4	2,4-Decadienal		Flavour and fragrance, present in fruits.
2420-56-6	10E,12Z-Octadecadienoic acid		NA
25152-83-4	2,4-Decadienal, (E,Z)-		Not specified
25152-84-5	2,4-Decadienal, (E,E)-		Not specified
26560-14-5	1,3,6,10-Dodecatetraene, 3,7,11trimethyl-, (Z,E)-		flavouring agent, natural pesticide
2777-58-4	6-Octadecenoic acid, methyl ester, (Z)-		NA
30364-38-6	Naphthalene, 1,2-dihydro-1,1,6trimethyl-		Not specified
3879-26-3	5,9-Undecadien-2-one, 6,10dimethyl-, (Z)-		Fragrance, flavouring agent
39702-28-8	Isopimara-9(11),15-diene		NA
39754-77-3	Tricosan-2-ol		Not specified
463-40-1	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-		Lubricant; other processing aids
474-62-4	Campesterol		NA
480-33-1	(-)-Mellein		NA
481-14-1	Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24Z)-		NA
498-07-7	.beta.-D-Glucofuranose, 1,6anhydro-		NA
506-21-8	Linoelaidic acid		NA
506-26-3	Gamolenic acid		Not specified
506-30-9	Eicosanoic acid		Lubricant; other processing aids
506-51-4	n-Tetracosanol-1		Biocide; colorant; f filler; intermediate; lubricant; odor agent; other processing aids
511-02-4	Naphthalene, decahydro-1,1,4a-trimethyl-6-methylene-5-(3methylene-4-pentenyl)-, [4aS(4a.alpha.,5.alpha.,8a.beta.)]-		NA
52207-99-5	cis-7,cis-11-Hexadecadien-1-yl acetate		NA
544-71-8	(9E,11E)-Octadecadienoic acid		NA
545-47-1	Lupeol		NA
55333-99-8	Eicosane, 7-hexyl-		NA



557-61-9	Octacosanol		Not specified
559-70-6	.beta.-Amyrin		NA
58670-89-6	2-Decyl-1-tetradecanol		Biocide; colorant; filler; intermediate; lubricant; odor agent; other processing aids
59-02-9	Vitamin E		Antioxidant
629-50-5	Tridecane		
629-59-4	Tetradecane		lubricant; odour agent
629-94-7	Heneicosane		NA
629-96-9	1-Eicosanol		Biocide; colorant; filler; intermediate; lubricant; odour agent; other processing aids
629-97-0	Docosane		Not specified
629-99-2	Pentacosane		Not specified
630-02-4	Octacosane		Emulsifier; surfactant; lubricant
630-03-5	Nonacosane		Not specified
630-04-6	Hentriacontane		Emulsifier; surfactant; lubricant
6386-38-5	Benzenepropanoic acid, 3,5bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester		Antioxidant; filler; light stabilizer; lubricant
638-67-5	Tricosane		NA
638-95-9	.alpha.-Amyrin		Not specified
646-31-1	Tetracosane		Emulsifier; surfactant; lubricant
7194-84-5	Heptatriacontane		NA
74685-30-6	5-Eicosene, (E)-		Not specified
7473-98-5	2-Hydroxy-iso-butyrophenone		Blowing agent; catalyst; colorant; crosslinking agent; initiator; lubricant; other processing aids
7616-22-0	.gamma.-Tocopherol		Not specified
83-47-6	.gamma.-Sitosterol		Not specified
83-48-7	Stigmasterol		Not specified
97-53-0	Eugenol		Colorant; odour agent
98-55-5	.alpha.-Terpineol		Odor agent
99-86-5	1,3-Cyclohexadiene, 1-methyl-4-(1methylethyl)-		Other processing aids

* Not official CAS Registry Numbers: "pseudo" identifiers created by NIST to link mass spectral records to corresponding chemical structures in the structure add-on files when an official CAS number was unavailable.



Yoghurt product

Both the yoghurt and pouch packaging sample types were found to contain a high number of total detectable chemical features (automatically deconvoluted peaks, no identity assigned), with the plastic packaging extracts exhibiting a higher average number of chemical features (8165) than the yoghurt extracts (6498). Across replicates, a total of 917 different chemical features (out of 8165) could be tentatively identified in the plastic extract based on their spectral similarity to library compounds (percentage match to NIST23 spectra >80 %) (Table A4). For the yoghurt extracts, a total of 656 chemical features were tentatively identified across the replicate samples (Table A5). After RT alignment within the dataset, exclusion of background chemicals, and consolidation of duplicate chemical identifiers, the replicate plastic pouch extracts were found to contain an average of 441 tentatively identified compounds, with the replicate yoghurt extracts containing an average of 357 tentatively identified compounds. A total of 111 tentatively identified compounds were found in both the packaging and yoghurt samples (Figure 7). These compounds were further examined to assess their relevance in plastic materials generally. Cross referencing with the PlastChem database, an inventory of chemicals known to be used in or found in plastics, revealed that 28 of the 111 common chemicals to the packaging and yoghurt are potentially plastic related (Table 3). Again, it is important to note that the presence of these compounds in both samples does not necessarily confirm that they have leached from the packaging material (for the reasons outlined above). Owing to the non-target screening approached used for these analyses, the identification of the compounds is considered to be tentative unless standards are used for confirmation.

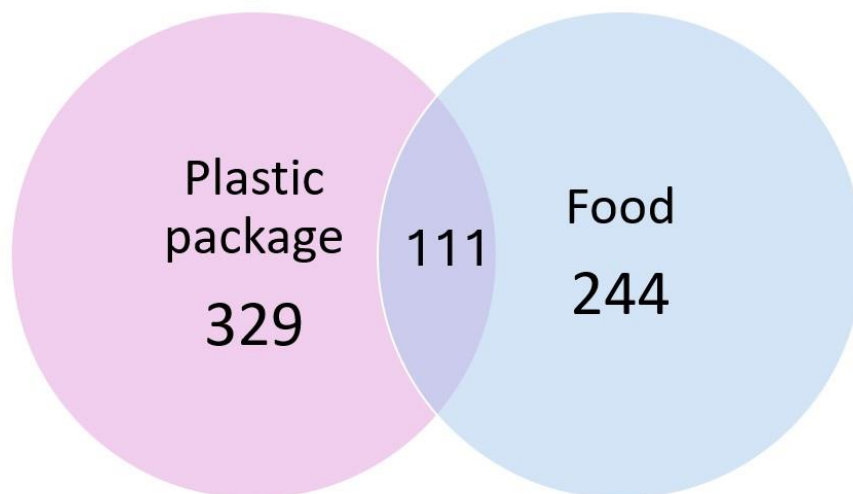


Figure 7: VENN diagram showing number of tentatively identified chemical features in the plastic packaging extracts, in the fruit foodstuff, and those common to both matrices.



Table 3: List of 111 chemicals tentatively identified both in the plastic package and in the foodstuff. The compounds marked as purple are those that are known to be used in or have been found in plastics according to PlastChem database (Monclús et al. 2025), while those marked in grey are those not present in the database. NA = not applicable.

CAS	Name	Identified as plastic chemical	Use
1000131-00-4*	13-Tetradecene-11-yn-1-ol		NA
1000190-45-8*	Acetic acid, 3-acetoxy-1-(2-acetoxy-1-methyl-ethyl)-2-methyl-propyl ester		NA
1000215-29-0*	cis-3-Methyl-endo-tricyclo[5.2.1.0(2.6)]decane		NA
1000309-18-4*	Sulfurous acid, butyl heptadecyl ester		NA
1000336-54-6*	Butyl 9,12,15-octadecatrienoate		NA
1000382-54-3*	Carbonic acid, eicosyl vinyl ester		NA
1000513-01-3*	Epilupeol; 20(29)-Lupen-3alpha-ol (isomer 1)		NA
1002-84-2	Pentadecanoic acid		Lubricant; other processing aids
10032-13-0	Butanoic acid, 3-methyl-, hexyl ester		NA
1010215-28-0*	2-Methylbicyclo[3.2.1]octane		NA
1014-60-4	Benzene, 1,3-bis(1,1-dimethylethyl)-		Non intentionally added substance; degradation product
105-60-2	Caprolactam		Catalyst; colorant; filler; intermediate monomer; other processing aids; plasticizer; solvent
110-34-9	Hexadecanoic acid, 2-methylpropyl ester		NA
111-06-8	Hexadecanoic acid, butyl ester		Lubricant
111-61-5	Octadecanoic acid, ethyl ester		NA
1117-52-8	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (E,E)-		NA
112-12-9	2-Undecanone		NA
112-39-0	Hexadecanoic acid, methyl ester		Biocide; colorant; filler; intermediate; lubricant; odour agent; other processing aids



112-63-0	9,12-Octadecadienoic acid (Z,Z)-, methyl ester		NA
1129-90-4	Cyclododecyne		NA
118-65-0	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4Z,9S*)]-		NA
1191-41-9	9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-		NA
1215128-07-6	6-Methyl-4-heptenyl pentanoate		NA
122-99-6	Ethanol, 2-phenoxy-		Antistatic agent; biocide; colorant; filler; intermediate; light stabilizer; lubricant; odour agent; other processing aids; plasticizer
123-69-3	Oxacycloheptadec-8-en-2-one, (8Z)-		NA
124-07-2	Octanoic acid		Biocide; colorant; filler; intermediate; lubricant; monomer; odour agent; other processing aids; plasticizer
128-37-0	Butylated Hydroxytoluene		Antioxidant; biocide; catalyst; colorant; crosslinking agent; filler; heat stabilizer; initiator; intermediate; light stabilizer; lubricant; odour agent; other processing aids; plasticizer
13058-52-1	Methyl 9-cis,11-trans-octadecadienoate		NA
13126-39-1	cis-13-Octadecenoic acid		NA
134-96-3	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-		NA
143-07-7	Dodecanoic acid		Biocide; colorant; filler; intermediate; lubricant; monomer; odour agent; other processing aids
1472-09-9	Cyclopropane, octyl-		NA
14722-40-8	1,15-Pentadecanediol		NA
150-86-7	Phytol		NA
1560-98-1	Octacosane, 2-methyl-		NA
1561-02-0	2-Methylhexacosane		NA
17643-36-6	9-Decyn-1-ol		NA
18435-45-5	1-Nonadecene		NA
18829-56-6	2-Nonenal, (E)-		NA
18835-32-0	1-Tricosene		NA
18835-33-1	1-Hexacosene		NA



18835-35-3	Nonacos-1-ene		NA
20290-75-9	Stearidonic acid		NA
20675-95-0	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol		NA
2277-16-9	4-Nonenal, (E)-		NA
2345-28-0	2-Pentadecanone		NA
2363-88-4	2,4-Decadienal		NA
2416-20-8	Hexadecenoic acid, Z-11-		NA
2425-77-6	1-Decanol, 2-hexyl-		Biocide; colorant; filler; intermediate; lubricant; odour agent; other processing aids
24252-85-5	1,4,8-Dodecatriene, (E,E,E)-		NA
2553-17-5	9-Oxononanoic acid		NA
2774-84-7	10-Undecyn-1-ol		NA
2777-58-4	6-Octadecenoic acid, methyl ester, (Z)-		NA
295-63-6	1,6,11-Trioxacyclopentadecane		NA
301-00-8	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-		NA
334-48-5	n-Decanoic acid		Biocide; catalyst; colorant; crosslinking agent; filler; initiator; lubricant; monomer; other processing aids
34450-18-5	17-Octadecynoic acid		NA
36653-82-4	1-Hexadecanol		Biocide; catalyst; colorant; crosslinking agent; filler; initiator; intermediate; light stabilizer; lubricant; monomer; odour agent; other processing aids; plasticizer; viscosity modifier
3796-70-1	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-		NA
3879-26-3	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-		NA
463-40-1	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-		Lubricant; other processing aids
474-62-4	Campesterol		NA
474-63-5	Ergosta-5,24(28)-dien-3-ol, (3.beta.)-		NA
474-77-1	Cholest-5-en-3-ol, (3.alpha.)-		NA
481-14-1	Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24Z)-		NA



487-11-6	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-		NA
497-32-5	Bicyclo[2.2.1]heptane, 2,2-dimethyl-5-methylene-		NA
498-02-2	Apocynin		NA
506-12-7	Heptadecanoic acid		Lubricant; other processing aids
506-17-2	cis-Vaccenic acid		NA
506-51-4	n-Tetracosanol-1		Biocide; colorant; filler; intermediate; lubricant; odour agent; other processing aids
544-35-4	Linoleic acid ethyl ester		NA
544-63-8	Tetradecanoic acid		Filler; lubricant; monomer; odour agent; other processing aids
544-71-8	(9E,11E)-Octadecadienoic acid		NA
54889-47-3	Pentane, 2,2'-[ethylidenebis(oxy)]bis-		NA
55255-56-6	Phenanthrene, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl-		NA
557-61-9	Octacosanol		NA
559-70-6	.beta.-Amyrin		NA
57-11-4	Octadecanoic acid		Antistatic agent; Biocide; catalyst; colorant; crosslinking agent; filler; intermediate; light stabilizer; lubricant; monomer; odour agent; other processing aids; plasticizer
5876-87-9	1,11-Dodecadiene		NA
59-02-9	Vitamin E		Antioxidant
593-49-7	Heptacosane		Emulsifier
60-12-8	Phenylethyl Alcohol		Biocide; colorant; intermediate; odour agent; other processing aids
6100-74-9	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-		NA
6114-18-7	(E)-9-Octadecenoic acid ethyl ester		NA
61886-64-4	3-Octadecyne		NA
621-59-0	Benzaldehyde, 3-hydroxy-4-methoxy-		NA
62238-24-8	Spiro[2.4]heptane, 1,5-dimethyl-6-methylene-		NA
62338-27-6	1,5,9,11-Tridecatetraene, 12-methyl-, (E,E)-		NA



628-97-7	Hexadecanoic acid, ethyl ester		NA
629-96-9	1-Eicosanol		Biocide; colorant; filler; intermediate; lubricant; odour agent; other processing aids
629-99-2	Pentacosane		NA
630-02-4	Octacosane		Emulsifier; surfactant; lubricant
630-03-5	Nonacosane		NA
630-04-6	Hentriacontane		Emulsifier; surfactant; lubricant
638-95-9	.alpha.-Amyrin		NA
65-85-0	Benzoic acid		Antioxidant; biocide; catalyst; colorant; crosslinking agent; filler; heat stabilizer; initiator; intermediate; lubricant; monomer; odor agent; other processing aids; plasticizer
659-70-1	Butanoic acid, 3-methyl-, 3-methylbutyl ester		NA
6627-88-9	Phenol, 2,6-dimethoxy-4-(2-propenyl)-		NA
7150-55-2	1-Butanone, 4-chloro-1-(4-hydroxyphenyl)-		NA
7212-91-1	Stigmasta-7,24(28)-dien-3-ol, (3.beta.,5.alpha.)-		NA
74663-68-6	3-Tetradecen-5-yne, (Z)-		NA
74744-37-9	2-Dodecen-4-yne, (Z)-		NA
765-13-9	1-Pentadecyne		NA
82253-09-6	7-Propylidene-bicyclo[4.1.0]heptane		NA
82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione		Non intentionally added substance; degradation product
83-47-6	.gamma.-Sitosterol		NA
83-48-7	Stigmasterol		NA
947-19-3	Methanone, (1-hydroxycyclohexyl)phenyl-		Catalyst; colorant; crosslinking agent; filler; initiator; intermediate; other processing aids; plasticizer
96-76-4	2,4-Di-tert-butylphenol		Antioxidant; intermediate; light stabilizer; lubricant
97-53-0	Eugenol		Colorant; odour agent

* Not official CAS Registry Numbers: “pseudo” identifiers created by the National Institute for Standards and Technology (NIST) to link mass spectral records to corresponding chemical structures in the structure add-on files when an official CAS number was unavailable.



4 Conclusion and recommendations

This pilot study represents one of the first attempts to assess the migration of MP and plastic-associated chemicals from packaging material into infant foodstuffs. The results provide evidence for the presence of MPs in a commercially available fruit-based product and a dairy-based product designed for infant consumption in the form of single use, disposable pouches. Across the three replicate foodstuff subsamples analysed for each product, MP concentrations were higher and had a different polymer composition than the MP found in the procedural blanks, indicating that the detected particles originate primarily from the products rather than from laboratory contamination. A range of MP polymer types were identified, with PE being the main polymer detected across both food matrices in almost equal quantity. The occurrence of PE is consistent with its use as the inner food-contact packaging material, suggesting that abrasion or degradation of the packaging may contribute to the MP content in the foodstuff. However, PE is also one of the most widely used polymers globally and may have entered the food product during production. Furthermore, the spectral fingerprint of PE can overlap with that of lipids commonly present in processed food items, meaning that its identification in this context should be considered tentative. It should therefore be noted that the total MP values reported in this study may be overestimated if some of the PE identifications represent false positives. The presence of other polymers appears to reflect contamination from other points in the processing and manufacturing chain, while PA might have resulted from laboratory contamination. Additional studies investigating the MP content of the foodstuffs prior to being placed in the packaging, ideally a various point along the production chain are required to assess if the packaging is the primary source of MP contamination observed in infant food products, or whether other steps in the production chain are important contributors.

Chemical analysis of the foodstuffs and their respective packaging revealed a higher number of total and tentatively identified chemicals in the plastic packaging than in the corresponding foodstuff for both products. Of these, 81 chemicals were identified in both the fruit product and corresponding packaging, with 53 of the chemicals identified as being potentially used in plastic or demonstrated to be associated with plastic. Similarly, 111 chemicals were identified both in the yoghurt product and corresponding packaging, with 28 of the chemicals identified as being potentially plastic related. The yoghurt appears to contain fewer chemicals in common with its packaging material than in the fruit, but it is important to consider that tentative identification could only be allocated to a relatively small proportion of the total chemical features observed in all the foodstuff and packaging products. Drawing strong conclusions that the fruit-based product is more likely to take on chemicals from the packaging is not recommended, as the picture may change if all chemicals could be tentatively identified in each sample type. It is important to highlight that the presence of the chemicals in the foodstuff does not necessarily confirm migration from packaging, and their presence may derive from other steps along the product production process, while migration of contaminant chemicals present in the foodstuff to the packaging may occur (essentially the foodstuff may contaminate the packaging). Either way, the presence of these chemicals in the final fruit and yoghurt products is clearly demonstrated by the study conducted here. Considering both products a total of 189 chemicals were tentatively identified in both packaging and the foodstuff, among these 163 were uniquely tentatively identified while 26 chemicals (reported in Table A6) were common to both products. As with MP, performing chemical analysis of the foodstuffs along the production chain may help to clarify the origin of the tentatively identified chemicals and assess their potential relevance for food safety. Similarly, conducting additional migration studies using pristine packaging will help to clarify uncertainty about the possible migration of chemical contaminants already present in the foodstuffs into the inner surface PE layer of the packaging material. Furthermore, to gain an insight into the potential human health implications of



these findings it is recommended that a hazard assessment is conducted on the 163 uniquely tentatively identified chemicals and MP observed across the two types of packaging and the two foodstuffs.

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Table A1: Summary of polymer composition and size of detected MP in analyzed subsamples.

Product and g of foodstuff per pouch	Sample ID	Sample wet weight (g)	Digestate (mL)	Subsample of digestate analysed with μ Raman (mL)	PE	PA	PP	PES	PS	EVA	PNT	SIS	PBT	20-50 (μ m)	50-110 (μ m)	110-300 (μ m)	>300 (μ m)	Sum MP
Fruit puree 113 g	Sample 1	10	55	1	6	6	0	0	0	1	1	1	0	13	2	0	0	15
	Sample 2	10	67	1	3	5	0	0	0	0	1	0	4	11	1	1	0	13
	Sample 3	10	71	1	12	8	6	0	0	0	0	0	0	24	1	1	0	26
	Blank 1	NA	49	1	0	2	0	0	4	0	0	0	0	5	1	0	0	6
	Blank 2	NA	36	1	2	5	0	0	0	0	0	0	0	3	4	0	0	7
	Blank 3	NA	36	1	0	0	0	0	3	0	0	0	0	3	0	0	0	3
Yoghurt 99 g	Sample 1	10	60	1	5	0	6	0	0	0	0	0	0	10	1	0	0	11
	Sample 2	10	60	1	5	0	0	0	0	0	0	0	0	5	0	0	0	5
	Sample 3	10	60	1	9	1	0	1	0	0	0	0	0	11	0	0	0	11
	Blank 1	NA	60	1	1	0	1	0	0	0	0	0	0	2	0	0	0	2
	Blank 2	NA	60	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	Blank 3	NA	60	1	0	0	0	0	0	0	0	0	1	1	0	0	0	1

**Table A2:** List of chemicals tentatively identified in the fruit puree package.

CAS number	Name
480-33-1	(-)-Mellein
193695-14-6	(1R,2R,5R,E)-7-Ethylidene-1,2,8,8-tetramethylbicyclo[3.2.1]octane
36577-33-0	(1R,3aS,8aS)-7-Isopropyl-1,4-dimethyl-1,2,3,3a,6,8a-hexahydroazulene
24738-48-5	(2E,4E)-2,4-Dodecadienoic acid
125456-63-5	(2E,6E,10E)-3,7,11,15-Tetramethylhexadeca-2,6,10,14-tetraen-1-yl formate
544-71-8	(9E,11E)-Octadecadienoic acid
53585-13-0	(E)-1-Methyl-4-(6-methylhept-5-en-2-ylidene)cyclohex-1-ene
638-95-9	.alpha.-Amyrin
21391-99-1	.alpha.-Calacorene
20129-39-9	.alpha.-Corocalene
98-55-5	.alpha.-Terpineol
559-70-6	.beta.-Amyrin
498-07-7	.beta.-D-Glucopyranose, 1,6-anhydro-
148-03-8	.beta.-Tocopherol
83-47-6	.gamma.-Sitosterol
7616-22-0	.gamma.-Tocopherol
392721-71-0	1-(2-Acetyloxy-5-methylphenyl)propan-1-one
1000357-25-8*	1, 1, 5-Trimethyl-1, 2-dihydronaphthalene
21964-49-8	1,13-Tetradecadiene
14811-95-1	1,19-Eicosadiene
643-93-6	1,1'-Biphenyl, 3-methyl-
613-37-6	1,1'-Biphenyl, 4-methoxy-
644-08-6	1,1'-Biphenyl, 4-methyl-
1000305-38-0*	1,1-Dichloronon-1-ene
16204-36-7	1,2,4,5-Tetroxane, 3,3,6,6-tetraphenyl-
26560-14-5	1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-
137-89-3	1,3-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester
99-86-5	1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-
126-11-4	1,3-Propanediol, 2-(hydroxymethyl)-2-nitro-
10395-09-2	1,3-Propanediol, 2-dodecyl
2717-39-7	1,4,5,8-Tetramethylnaphthalene
88-58-4	1,4-Benzenediol, 2,5-bis(1,1-dimethylethyl)-
1113-21-9	1,6,10,14-Hexadecatetraen-3-ol, 3,7,11,15-tetramethyl-, (E,E)-
40716-66-3	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-
295-63-6	1,6,11-Trioxacyclopentadecane
2420-56-6	10E,12Z-Octadecadienoic acid
128792-46-1	11-Dodecen-1-ol trifluoroacetate



85763-57-1	11-Methyldodecanol
52380-33-3	11-Octadecenoic acid, methyl ester
6971-40-0	17-Pentatriacontene
94-46-2	1-Butanol, 3-methyl-, benzoate
21078-65-9	1-Decanol, 2-ethyl-
2425-77-6	1-Decanol, 2-hexyl-
45235-48-1	1-Decanol, 2-octyl-
1000333-91-9*	1-Docosanol, methyl ether
110225-00-8	1-Dodecanol, 2-hexyl-
5333-42-6	1-Dodecanol, 2-octyl-
112-41-4	1-Dodecene
629-96-9	1-Eicosanol
567040	1-Eicosene
28580-43-0	1H-Cycloprop[e]azulene, decahydro-1,1,4,7-tetramethyl-, [1aR-(1a.alpha.,4.beta.,4a.beta.,7.beta.,7a.beta.,7b.alpha.)]-
2004-39-9	1-Heptacosanol
10042-59-8	1-Heptanol, 2-propyl-
506-52-5	1-Hexacosanol
2471-83-2	1H-Indene, 1-ethylidene-
596-84-9	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3.alpha.,4a.beta.,6a.alpha.,10a.beta.,10b.alpha.)]-
1227-93-6	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3S-(3.alpha.,4a.alpha.,6a.beta.,10a.alpha.,10b.beta.)]-
237742-62-0	1-Methoxyoctacosane
1438-62-6	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-.alpha.,5,5,8a-tetramethyl-2-methylene-, [1S-[1.alpha.(R*),4a.beta.,8a.alpha.]]-
18435-45-5	1-Nonadecene
112-92-5	1-Octadecanol
1000406-29-3*	1-Octadecanol, methyl ether
112-88-9	1-Octadecene
735273	1-Octanol, 2-butyl-
29833-69-0	1-Pentadecene, 2-methyl-
13601-88-2	1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-, [1R-(1.alpha.,4a.beta.,10a.alpha.)]-
593-50-0	1-Triacontanol
450350	1-Tricosanol
18835-32-0	1-Tricosene
1000292-44-2*	2-Bromopropionic acid, pentadecyl ester
1000486-97-7*	2,4,2',4'-Tetramethyl-biphenyl
19687-22-0	2,4,6-Tris(1,1-dimethylethyl)-4-methylcyclohexa-2,5-dien-1-one
2363-88-4	2,4-Decadienal
25152-84-5	2,4-Decadienal, (E,E)-



25152-83-4	2,4-Decadienal, (E,Z)-
5910-87-2	2,4-Nonadienal, (E,E)-
55162-56-6	2,5-Cyclohexadien-1-one, 4,4-dimethyl-3-phenyl-
719-22-2	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-
61691-98-3	2,6,10,14-Hexadecatetraen-1-ol, 3,7,11,15-tetramethyl-, acetate, (E,E,E)-
17909-77-2	2,6,9,11-Dodecatetraenal, 2,6,10-trimethyl-, (E,E,E)-
13187-99-0	2-Bromo dodecane
23726-93-4	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)-
51655-65-3	2-Butyl-1-decene
2497-25-8	2-Decenal, (Z)-
58670-89-6	2-Decyl-1-tetradecanol
1000368-55-9*	2-Hexyldodecyl acetate
7473-98-5	2-Hydroxy-iso-butyrophenone
52254-38-3	2-Methyl-1-tetradecene
10522-26-6	2-Methyl-1-undecanol
64183-52-4	2-Methyl-E-7-hexadecene
1560-72-1	2-Methyltriacontane
1653-34-5	2-Pentadecanol
195194-80-0	2-Piperidinone, N-[4-bromo-n-butyl]-
7779-31-9	2-Propenoic acid, 2-methyl-, 3,3,5-trimethylcyclohexyl ester
10059-13-9	2-Undecanethiol, 2-methyl-
112-12-9	2-Undecanone
203499-08-5	3-((1S,5S,6R)-2,6-Dimethylbicyclo[3.1.1]hept-2-en-6-yl)propanal
6390-69-8	3,3',5,5'-Tetra-tert-butylbiphenyl-2,2'-diol
14035-33-7	3,5-di-tert-Butyl-4-hydroxyacetophenone
20170-32-5	3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid
74685-33-9	3-Eicosene, (E)-
34303-81-6	3-Hexadecene, (Z)-
14167-66-9	3-Methylheptacosane
6902-54-1	3-Methylpentacosane
7206-19-1	3-Octadecene, (E)-
41446-68-8	3-Tetradecene, (E)-
74630-49-2	3-Undecene, 7-methyl-, (Z)-
96168-15-9	4,8,12,16-Tetramethylheptadecan-4-olide
2277-16-9	4-Nonenal, (E)-
41446-78-0	4-Tetradecene, (E)-
41446-65-5	4-Tetradecene, (Z)-
1000245-47-6*	4-Trifluoroacetoxytetradecane
74645-87-7	4-Undecene, 3-methyl-, (Z)-
74630-57-2	4-Undecene, 4-methyl-, (Z)-
74630-69-6	4-Undecene, 5-methyl-, (Z)-



1117-52-8	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (E,E)-
689-67-8	5,9-Undecadien-2-one, 6,10-dimethyl-
3796-70-1	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-
3879-26-3	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-
74685-30-6	5-Eicosene, (E)-
7206-21-5	5-Octadecene, (E)-
41446-66-6	5-Tetradecene, (E)-
41446-62-2	5-Tetradecene, (Z)-
2387-68-0	6,10-Dodecadien-1-yn-3-ol, 3,7,11-trimethyl-
2277-19-2	6-Nonenal, (Z)-
2777-58-4	6-Octadecenoic acid, methyl ester, (Z)-
41446-64-4	6-Tetradecene, (E)-
1010548-12-8*	7-Acetoxy-3,4-dimethyl-1-indanone
35507-09-6	7-Hexadecene, (Z)-
1000374-20-4*	7-Hydroxyfarnesen
21061-10-9	8,11,14-Eicosatrienoic acid, methyl ester, (Z,Z,Z)-
13038-47-6	9,11-Octadecadienoic acid, methyl ester, (E,E)-
463-40-1	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
112-63-0	9,12-Octadecadienoic acid (Z,Z)-, methyl ester
112-62-9	9-Octadecenoic acid (Z)-, methyl ester
112-79-8	9-Octadecenoic acid, (E)-
2553-17-5	9-Oxononanoic acid
83-32-9	Acenaphthene
506-32-1	Arachidonic acid
50-78-2	Aspirin
661-19-8	Behenic alcohol
18299-85-9	Behenyl acrylate
4537-15-9	Benzene, (1-butylheptyl)-
4534-50-3	Benzene, (1-butylnonyl)-
2719-63-3	Benzene, (1-butylloctyl)-
4536-87-2	Benzene, (1-ethylnonyl)-
4534-52-5	Benzene, (1-ethylundecyl)-
182625	Benzene, (1-hexylheptyl)-
4536-88-3	Benzene, (1-methyldecyl)-
4534-53-6	Benzene, (1-methyldodecyl)-
2719-61-1	Benzene, (1-methylundecyl)-
2719-62-2	Benzene, (1-pentylheptyl)-
4537-14-8	Benzene, (1-pentylhexyl)-
4534-49-0	Benzene, (1-pentylloctyl)-
2719-64-4	Benzene, (1-propylnonyl)-
4536-86-1	Benzene, (1-propylloctyl)-



101-68-8	Benzene, 1,1'-methylenebis[4-isocyanato-
487-11-6	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-
1014-60-4	Benzene, 1,3-bis(1,1-dimethylethyl)-
6386-38-5	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester
2082-79-3	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester
61142-06-1	Benzocyclodecene, tetradecahydro-
6789-88-4	Benzoic acid, hexyl ester
119-61-9	Benzophenone
120-51-4	Benzyl Benzoate
88034-74-6	Bergamotol, Z-.alpha.-trans-
17065-18-8	Bicyclo[2.1.0]pentane, 1,4-dimethyl-
464-17-5	Bicyclo[2.2.1]hept-2-ene, 1,7,7-trimethyl-
547-60-4	Bicyclo[3.1.1]heptan-3-one, 2,6,6-trimethyl-, (1.alpha.,2.alpha.,5.alpha.)-
74792-79-3	Borane, [1,2-bis(1-methylethyl)butyl]bis(1-methylethyl)-
10032-15-2	Butanoic acid, 2-methyl-, hexyl ester
109-21-7	Butanoic acid, butyl ester
2639-63-6	Butanoic acid, hexyl ester
1000336-54-1*	Butyl 9,12-octadecadienoate
1000360-29-8*	Butyl 9-decenoate
128-37-0	Butylated Hydroxytoluene
58-08-2	Caffeine
474-62-4	Campesterol
1000383-16-0*	Carbonic acid, decyl undecyl ester
1000383-25-7*	Carbonic acid, decyl vinyl ester
1000382-54-4*	Carbonic acid, octadecyl vinyl ester
87-44-5	Caryophyllene
18252-46-5	cis-.alpha.-Bergamotene
52207-99-5	cis-7,cis-11-Hexadecadien-1-yl acetate
72937-55-4	cis-Calamenene
5392-40-5	Citral
16539-09-6	Cyclodecane, octyl-
1000151-22-6*	Cyclodocosane, ethyl-
296-56-0	Cycloeicosane
295-65-8	Cyclohexadecane
7045-67-2	Cyclohexane, 2-ethyl-1,3-dimethyl-
4292-75-5	Cyclohexane, hexyl-
3964-66-7	Cyclohexene,1-hexyl-
297-24-5	Cyclooctacosane
1000151-22-5*	Cyclooctadecane, ethyl-
1000556-71-2*	Cyclopent-2-enone, 5-methylene-2,3,4,4-tetrame
55255-85-1	Cyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediy]bis-



55429-35-1	Cyclopentane, 1,1'-[4-(3-cyclopentylpropyl)-1,7-heptanediyl]bis-
62199-51-3	Cyclopentane, 1-pentyl-2-propyl-
61142-65-2	Cyclopentane, 3-hexyl-1,1-dimethyl-
4457-00-5	Cyclopentane, hexyl-
2882-98-6	Cyclopentane, nonyl-
74630-58-3	Cyclopropane, 1-hexyl-2-propyl-, cis-
297-03-0	Cyclotetracosane
59739-63-8	Damascenone,(Z)-beta-
2050-77-3	Decane, 1-iodo-
192823-15-7	Decane, 2,3,5,8-tetramethyl-
110-42-9	Decanoic acid, methyl ester
50894-66-1	Di-epi-.alpha.-cedrene
96-26-4	Dihydroxyacetone
101-81-5	Diphenylmethane
10191-41-0	dl-.alpha.-Tocopherol
629-97-0	Docosane
13475-76-8	Docosane, 11-butyl-
55401-55-3	Docosane, 11-decyl-
1000406-31-9*	Docosane, 1-iodo-
77536-30-2	Docosane, 2,4-dimethyl-
55373-86-9	Docosane, 7-hexyl-
108698-02-8	Docosapentaenoic Acid methyl ester
1000351-83-1*	Docosyl heptafluorobutyrate
1000406-39-7*	Docosyl heptyl ether
1000406-37-9*	Docosyl nonyl ether
1000351-80-9*	Docosyl pentafluoropropionate
112-40-3	Dodecane
31295-56-4	Dodecane, 2,6,11-trimethyl-
61141-72-8	Dodecane, 4,6-dimethyl-
10233-13-3	Dodecanoic acid, 1-methylethyl ester
2874-74-0	Dodecanoic acid, 2-methyl-
544-85-4	Dotriacontane
1000406-32-4*	Dotriacontane, 1-iodo-
1720-11-2	Dotriacontane, 2-methyl-
1000351-84-2*	Dotriacontyl heptafluorobutyrate
1000385-71-0*	E-11-Tetradecen-1-ol trifluoroacetate
1000130-97-9*	E-15-Heptadecenal
1000130-92-0*	E-7-Octadecene
54833-23-7	Eicosane, 10-methyl-
75163-98-3	Eicosane, 2,4-dimethyl-
55333-99-8	Eicosane, 7-hexyl-



4443-61-2	Eicosane, 9-cyclohexyl-
13475-77-9	Eicosane, 9-octyl-
506-30-9	Eicosanoic acid
1000406-33-0*	Eicosyl isobutyl ether
1000406-37-8*	Eicosyl nonyl ether
1000406-38-8*	Eicosyl octyl ether
4651-51-8	Ergost-5-en-3-ol, (3.beta.)-
140-67-0	Estragole
2136-72-3	Ethanol, 2-(octadecyloxy)-
122-99-6	Ethanol, 2-phenoxy-
1009-61-6	Ethanone, 1,1'-(1,4-phenylene)bis-
97-53-0	Eugenol
83637-40-5	Farnesene epoxide, E-
506-26-3	Gamolenic acid
37839-64-8	Guaiadiene, 6,9-
629-94-7	Heneicosane
6418-47-9	Heneicosane, 3-methyl-
25117-37-7	Heneicosane, 5-methyl-
1000351-83-8*	Heneicosyl heptafluorobutyrate
630-04-6	Hentriacontane
61868-03-9	Heptadecane, 2,3-dimethyl-
18344-37-1	Heptadecane, 2,6,10,14-tetramethyl-
54833-48-6	Heptadecane, 2,6,10,15-tetramethyl-
6418-44-6	Heptadecane, 3-methyl-
506-12-7	Heptadecanoic acid
7194-84-5	Heptatriacontane
1000406-40-0*	Heptyl octacosyl ether
1000406-39-5*	Heptyl octadecyl ether
55429-83-9	Hexacosane, 9-octyl-
1000351-83-3*	Hexacosyl heptafluorobutyrate
1010406-38-1*	Hexacosyl nonyl ether
1000406-42-3*	Hexacosyl pentyl ether
1081180	Hexadecane, 1-chloro-
504-44-9	Hexadecane, 2,6,11,15-tetramethyl-
1560-92-5	Hexadecane, 2-methyl-
25117-26-4	Hexadecane, 4-methyl-
921-47-1	Hexane, 2,3,4-trimethyl-
626-82-4	Hexanoic acid, butyl ester
6378-65-0	Hexanoic acid, hexyl ester
630-06-8	Hexatriacontane
1000351-89-0*	Hexatriacontyl pentafluoropropionate



17071-54-4	Hexyl octyl ether
16930-96-4	Hexyl tiglate
1000406-33-4*	Isobutyl octacosyl ether
1000406-33-7*	Isobutyl tetratriacontyl ether
1000406-33-5*	Isobutyl triacontyl ether
95910-36-4	isolekene
39702-28-8	Isopimara-9(11),15-diene
10482-56-1	L-.alpha.-Terpineol
506-21-8	Linoelaidic acid
545-47-1	Lupeol
1000336-35-1*	Methyl 8,11,14-heptadecatrienoate
119-36-8	Methyl salicylate
112-61-8	Methyl stearate
1000406-30-1*	Methyl tetratriacontyl ether
1000406-29-9*	Methyl triacontyl ether
91-20-3	Naphthalene
2809-64-5	Naphthalene, 1,2,3,4-tetrahydro-5-methyl-
3031-15-0	Naphthalene, 1,2,3,4-tetramethyl-
30364-38-6	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-
573-98-8	Naphthalene, 1,2-dimethyl-
575-41-7	Naphthalene, 1,3-dimethyl-
2131-42-2	Naphthalene, 1,4,6-trimethyl-
571-61-9	Naphthalene, 1,5-dimethyl-
2245-38-7	Naphthalene, 1,6,7-trimethyl-
575-43-9	Naphthalene, 1,6-dimethyl-
483-78-3	Naphthalene, 1,6-dimethyl-4-(1-methylethyl)-
2027-17-0	Naphthalene, 2-(1-methylethyl)-
581-42-0	Naphthalene, 2,6-dimethyl-
91-57-6	Naphthalene, 2-methyl-
511-02-4	Naphthalene, decahydro-1,1,4a-trimethyl-6-methylene-5-(3-methylene-4-pentenyl)-, [4aS-(4a.alpha.,5.alpha.,8a.beta.)]-
24932-56-7	N-Cyclohexyl-2,2-diphenylacetamide
18835-35-3	Nonacos-1-ene
630-03-5	Nonacosane
14167-67-0	Nonacosane, 3-methyl-
75163-99-4	Nonadecane, 2,3-dimethyl-
40710-32-5	Nonahexacontanoic acid
1000406-38-2*	Nonyl octacosyl ether
1000406-38-0*	Nonyl tetracosyl ether
1000406-37-6*	Nonyl tetradecyl ether
1000336-77-8*	n-Propyl 9,12-octadecadienoate



506-51-4	n-Tetracosanol-1
630-02-4	Octacosane
1560-98-1	Octacosane, 2-methyl-
557-61-9	Octacosanol
1010351-83-6*	Octacosyl heptafluorobutyrate
1000406-42-4*	Octacosyl pentyl ether
593-45-3	Octadecane
930-02-9	Octadecane, 1-(ethenyloxy)-
75163-97-2	Octadecane, 2,6-dimethyl-
1560-88-9	Octadecane, 2-methyl-
106-11-6	Octadecanoic acid, 2-(2-hydroxyethoxy)ethyl ester
1000406-38-7*	Octadecyl octyl ether
79392-43-1	Octadecyl trifluoroacetate
124-07-2	Octanoic acid
2035-99-6	Octanoic acid, 3-methylbutyl ester
1117-55-1	Octanoic acid, hexyl ester
1000351-89-1*	Octatriacontyl pentafluoropropionate
112-80-1	Oleic Acid
1000352-68-4*	Oleyl alcohol, trifluoroacetate
629-99-2	Pentacosane
2882-96-4	Pentadecane, 3-methyl-
52997-43-0	Pentadecane, 7-(bromomethyl)-
6165-40-8	Pentadecane, 7-methyl-
1002-84-2	Pentadecanoic acid
630-07-9	Pentatriacontane
1000406-42-6*	Pentyl dotriacontyl ether
1000406-42-5*	Pentyl triacontyl ether
377851	Phenol, 2,4,6-tris(1-methylethyl)-
120-95-6	Phenol, 2,4-bis(1,1-dimethylpropyl)-
97-54-1	Phenol, 2-methoxy-4-(1-propenyl)-
5912-86-7	Phenol, 2-methoxy-4-(1-propenyl)-, (Z)-
1988-89-2	Phenol, 4-(1-phenylethyl)-
5454-19-3	Propanoic acid, decyl ester
39007-93-7	Sesquirosefuran
2117-34-2	Silane, triethylmethoxy-
481-14-1	Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24Z)-
83-48-7	Stigmasterol
1000309-17-9*	Sulfurous acid, butyl dodecyl ester
1000309-18-3*	Sulfurous acid, butyl hexadecyl ester
1000309-18-5*	Sulfurous acid, butyl octadecyl ester
1000309-13-3*	Sulfurous acid, hexyl undecyl ester



1000309-12-6*	Sulfurous acid, pentadecyl 2-propyl ester
646-31-1	Tetracosane
55429-84-0	Tetracosane, 11-decyl-
55401-54-2	Tetracosane, 9-octyl-
1000351-83-7*	Tetracosyl heptafluorobutyrate
629-59-4	Tetradecane
25117-24-2	Tetradecane, 4-methyl-
1000156-09-4*	Tetrapentacontane, 1,54-dibromo-
14167-59-0	Tetratriacontane
14167-65-8	Tetratriacontane, 2-methyl-
1000351-84-1*	Tetratriacontyl heptafluorobutyrate
1000351-81-5*	Tetratriacontyl pentafluoropropionate
21145-77-7	Tonalid
13474-59-4	trans-.alpha.-Bergamotene
1000333-61-3*	trans-13-Octadecenoic acid, methyl ester
1000405-19-1*	trans-9-Octadecenoic acid, pentyl ester
638-68-6	Triacontane
1000406-32-3*	Triacontane, 1-iodo-
1000351-83-2*	Triacontyl heptafluorobutyrate
1000351-80-0*	Triacontyl pentafluoropropionate
39754-77-3	Tricosan-2-ol
638-67-5	Tricosane
41370-56-3	Tricyclo[4.4.0.0(2,7)]dec-8-ene-3-methanol, .alpha.,.alpha.,6,8-tetramethyl-, stereoisomer
629-50-5	Tridecane
6418-41-3	Tridecane, 3-methyl-
25117-31-1	Tridecane, 5-methyl-
19780-80-4	Tridecane, 7-methylene-
17312-77-5	Undecane, 2,3-dimethyl-
17301-32-5	Undecane, 4,7-dimethyl-
121-33-5	Vanillin
1203-21-0	Verbenyl acetate,trans-
59-02-9	Vitamin E

* Not official CAS Registry Numbers: "pseudo" identifiers created by NIST to link mass spectral records to corresponding chemical structures in the structure add-on files when an official CAS number was unavailable.

Table A1: List of chemicals tentatively identified in the fruit puree foodstuff

CAS number	Name
480-33-1	(-)-Mellein
1000306-71-8*	(2,3-Dimethyloxiranyl)methanol
78368-58-8	(2E,6E)-3,7,11-Trimethyldodeca-2,6,10-trien-1-yl dodecanoate



125456-63-5	(2E,6E,10E)-3,7,11,15-Tetramethylhexadeca-2,6,10,14-tetraen-1-yl formate
35854-86-5	(6Z)-Nonen-1-ol
544-71-8	(9E,11E)-Octadecadienoic acid
20675-95-0	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol
10030-73-6	(E)-Hexadec-9-enoic acid
1572-93-6	(R)-(-)-3-Methyl-2-butanol
102-94-3	(Z)-3-Phenyl-2-propenoic acid
638-95-9	.alpha.-Amyrin
14687-15-1	.alpha.-L-Galactopyranoside, methyl 6-deoxy-
1467-70-5	.alpha.-Oxo-2-furanacetic acid
98-55-5	.alpha.-Terpineol
559-70-6	.beta.-Amyrin
498-07-7	.beta.-D-Glucopyranose, 1,6-anhydro-
83-46-5	.beta.-Sitosterol
915-05-9	.beta.-Sitosterol acetate
148-03-8	.beta.-Tocopherol
83-47-6	.gamma.-Sitosterol
7616-22-0	.gamma.-Tocopherol
1000357-25-8*	1, 1, 5-Trimethyl-1, 2-dihydronaphthalene
13688-67-0	1,10-Undecadiene
1000365-58-6*	1,2,3,6-Tetrahydrobenzylalcohol, acetate
106-61-6	1,2,3-Propanetriol, 1-acetate
110-88-3	1,3,5-Trioxane
26560-14-5	1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-
18368-95-1	1,3,8-p-Menthatriene
36645-68-8	1,30-Triacontanediol
99-86-5	1,3-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-
22013-33-8	1,4-Benzodioxan-6-amine
824-46-4	1,4-Benzenediol, 2-methoxy-
7425-74-3	1,6-Anhydro-.beta.-D-glucofuranose
629-11-8	1,6-Hexanediol
62108-28-5	1,7-Nonadiene, 4,8-dimethyl-
13175-32-1	1,7-Octanediol
2420-56-6	10E,12Z-Octadecadienoic acid
112-43-6	10-Undecen-1-ol
112-45-8	10-Undecenal
35289-31-7	11-Dodecenol
53596-78-4	11-Dodecyn-1-ol acetate
629-98-1	13-Docosen-1-ol, (Z)-
58594-45-9	13-Octadecenal, (Z)-
286-99-7	13-Oxabicyclo[10.1.0]tridecane



1000131-00-4*	13-Tetradecene-11-yn-1-ol
1010144-57-9*	16-Heptadecenal
51326-51-3	1-Butanol, 4-[(tetrahydro-2H-pyran-2-yl)oxy]-
13942-77-3	1-Deoxy-d-arabitol
629-96-9	1-Eicosanol
1000484-40-4*	1-Ethynylcyclododecanol
49607-51-4	1H-1,2,4-Triazol-3-amine, 1-methyl-
18835-33-1	1-Hexacosene
1470-94-6	1H-Inden-5-ol, 2,3-dihydro-
1000316-44-9*	1H-Pyrazole-4-carboxylic acid
20845-34-5	1-Methyl-2-piperidinemethanol
1000522-25-6*	1-Methyl-4-(4-methylpent-3-en-1-yl)cyclohex-3-enecarbaldehyde (isomer 2)
18435-45-5	1-Nonadecene
143-08-8	1-Nonanol
112-92-5	1-Octadecanol
172008	1-Pentanol, 2,2-dimethyl-
34419-76-6	1-Propanamine, N,2-dimethyl-N-nitroso-
10192-32-2	1-Tetracosene
18835-32-0	1-Tricosene
26186-02-7	1-Tridecyne
220556-75-2	2-((8Z,11Z)-Heptadeca-8,11-dien-1-yl)-4,5-dihydrooxazole
5469-16-9	2(3H)-Furanone, dihydro-4-hydroxy-
1332747-95-1	2-(Hydroxymethyl)-3-methoxy-2H-furan-5-one
31297-34-4	2,3-Dihydro-4,5,7-trimethyl-2,3-dioxobenzofuran
2363-88-4	2,4-Decadienal
25152-84-5	2,4-Decadienal, (E,E)-
25152-83-4	2,4-Decadienal, (E,Z)-
1010142-19-7*	2,4-Pentadien-1-ol, 3-pentyl-, (2Z)-
1000150-21-6*	2,5-Cyclohexadiene, 1,4-diethyl-1,4-dimethyl-
15233-65-5	2,6-Dimethoxyhydroquinone
460-01-5	2,6-Dimethyl-1,3,5,7-octatetraene, E,E-
7494-34-0	26-Nor-5-cholesten-3.beta.-ol-25-one
624-48-6	2-Butenedioic acid (Z)-, dimethyl ester
77846-84-5	2-Cyclohexen-1-one, 4-hydroxy-3,5,6-trimethyl-4-(3-oxo-1-butenyl)-
58670-89-6	2-Decyl-1-tetradecanol
22073-04-7	2-Furancarboxylic acid, tetrahydro-3-methyl-5-oxo-
5989-33-3	2-Furanmethanol, 5-ethenyltetrahydro-.alpha.,.alpha.,5-trimethyl-, cis-
17675-99-9	2-Furanone, 3,4-dihydroxytetrahydro
1721-51-3	2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-
1121-84-2	2H-Pyran-2-one, tetrahydro-4-methyl-



7473-98-5	2-Hydroxy-iso-butyrophenone
3451-51-2	2-Methyl[1,3,4]oxadiazole
18829-56-6	2-Nonenal, (E)-
4899-74-5	2-Propanone, 1-hydroxy-3-(4-hydroxy-3-methoxyphenyl)-
1135-24-6	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-
14293-08-4	2-Pyrrolidinone, 5-(cyclohexylmethyl)-
55194-58-6	2-Undecanol palmitate
112-12-9	2-Undecanone
53448-07-0	2-Undecenal, E-
10210-17-0	3-(p-Hydroxyphenyl)-1-propanol
3142-58-3	3,3-Dimethyl-2,4-pentane dione
133610-00-1	3,3-Dimethyl-4-phenyl-4-penten-2-one
5803-57-6	3,4-Dihydroxy-5-methyl-dihydrofuran-2-one
22554-74-1	3,4-Furandiol, tetrahydro-, trans-
59643-68-4	3,5-Dimethyl-3-heptene
20170-32-5	3,5-di-tert-Butyl-4-hydroxyphenylpropionic acid
501-19-9	3-Allyl-6-methoxyphenol
29548-14-9	3-Cyclohexene-1-acetaldehyde, .alpha.,4-dimethyl-
6790-27-8	3-Dodecyne
102488-09-5	3-Hydroxy-.beta.-damascone
140235-34-3	3-Hydroxy-4-methoxy-4-oxobutanoic acid
645-08-9	3-Hydroxy-4-methoxybenzoic acid
1010430-01-2*	3-Methoxy-3-methylbutyl acetate
600-36-2	3-Pentanol, 2,4-dimethyl-
25110-61-6	3-Propylhexanoic acid
60212-32-0	3-Tetradecyne
60186-78-9	3-Tridecene
60212-30-8	3-Undecyne
134855-87-1	4-(1-Aminoethyl)phenol
27830-77-9	4,4,6-Trimethyltetrahydro-1,3-oxazin-2-one
1000399-10-0*	4,4'-bi-4H-pyran, 2,2',6,6'-tetrakis(1,1-dimethylethyl)-4,4'-dimethyl-
4441-57-0	4-Cyclohexyl-1-butanol
28564-83-2	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
1073-96-7	4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-
501-30-4	4H-Pyran-4-one, 5-hydroxy-2-(hydroxymethyl)-
6100-60-3	4-Methoxy-1,3-benzenediol
2277-16-9	4-Nonenal, (E)-
1516892	4-Vinylbenzene-1,2-diol
1000531-26-2*	5-(1-Hydroxyethyl)oxolan-2-one (isomer 1)
1917-64-2	5-(Methoxymethyl)furan-2-carbaldehyde
1000364-20-1*	5,5-Dimethyl-1,3-dioxane-2-ethanol, TBDMS derivative



3879-26-3	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-
10551-58-3	5-Acetoxyethyl-2-furaldehyde
52788-73-5	5-Docosyldihydrofuran-2(3H)-one
74685-30-6	5-Eicosene, (E)-
67-47-0	5-Hydroxymethylfurfural
2294-72-6	5-Undecyne
81265-03-4	6,9-Heptadecadiene
2777-58-4	6-Octadecenoic acid, methyl ester, (Z)-
42371-66-4	6-Tridecane
29210-77-3	7-Octene-2,6-diol, 2,6-dimethyl-
35216-11-6	7-Tetradecyne
31642-67-8	8-Nonenoic acid
13038-47-6	9,11-Octadecadienoic acid, methyl ester, (E,E)-
463-40-1	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
506-43-4	9,12-Octadecadien-1-ol, (Z,Z)-
2277-28-3	9,12-Octadecadienoic acid (Z,Z)-, 2,3-dihydroxypropyl ester
2566-97-4	9,12-Octadecadienoic acid, methyl ester, (E,E)-
7459-33-8	9,12-Octadecadienoyl chloride, (Z,Z)-
51937-00-9	9,12-Tetradecadien-1-ol, (Z,E)-
17309-05-6	9,15-Octadecadienoic acid, methyl ester, (Z,Z)-
25107-01-1	9-Methylbicyclo[3.3.1]nonane
112-62-9	9-Octadecenoic acid (Z)-, methyl ester
112-79-8	9-Octadecenoic acid, (E)-
1937-62-8	9-Octadecenoic acid, methyl ester, (E)-
20862-58-2	Acetic acid, 2-(coumarin-3-yl)-
498-02-2	Apocynin
621-59-0	Benzaldehyde, 3-hydroxy-4-methoxy-
123-08-0	Benzaldehyde, 4-hydroxy-
134-96-3	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-
156-38-7	Benzeneacetic acid, 4-hydroxy-
6386-38-5	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester
106148-64-5	Benzo[c][1,2,5]-thiadiazole, 4,5,6,7-tetramethyl-
496-16-2	Benzofuran, 2,3-dihydro-
1000375-33-5*	Benzoic acid, 2-(isopropyl)oxy-, methyl ester
50-30-6	Benzoic acid, 2,6-dichloro-
99-96-7	Benzoic acid, 4-hydroxy-
530-57-4	Benzoic acid, 4-hydroxy-3,5-dimethoxy-
84-73-1	Bis(2-hydroxyethyl) phthalate
110-15-6	Butanedioic acid
1583941	Butanedioic acid, 2-hydroxy-2-methyl-, (S)-
97-67-6	Butanedioic acid, hydroxy-, (S)-



10032-15-2	Butanoic acid, 2-methyl-, hexyl ester
600-18-0	Butanoic acid, 2-oxo-
1000336-54-1*	Butyl 9,12-octadecadienoate
77-94-1	Butyl citrate
474-62-4	Campesterol
57-88-5	Cholesterol
18252-46-5	cis-.alpha.-Bergamotene
29587-92-6	cis-1,2-Epoxy cyclodecane
13126-39-1	cis-13-Octadecenoic acid
52207-99-5	cis-7,cis-11-Hexadecadien-1-yl acetate
2416-19-5	cis-7-Hexadecenoic acid
1000405-15-0*	cis-9-Octadecenoic acid, propyl ester
506-17-2	cis-Vaccenic acid
141-16-2	Citronellyl butyrate
4651-54-1	Clionasterol acetate
359248	Cyclohexane, 1,1'-(2-methyl-1,3-propanediyl)bis-
62337-96-6	Cyclohexane, 1,1,2-trimethyl-3,5-bis(1-methylethenyl)-, (2.alpha.,3.alpha.,5.beta.)-
80-53-5	Cyclohexanemethanol, 4-hydroxy-.alpha.,.alpha.,4-trimethyl-
4668-64-8	Cyclohexanone, 2-isobutyl-
1255190	D-(+)-Ribonic acid .gamma.-lactone
2595-97-3	D-Allose
20736-25-8	Dihydrosyringenin
10191-41-0	dl-.alpha.-Tocopherol
66183-71-9	DL-Proline, 5-oxo-, ethyl ester
1114-34-7	d-Lyxose
629-97-0	Docosane
112-85-6	Docosanoic acid
26720-37-6	Docosanoic acid, hexyl ester
112-40-3	Dodecane
13151-85-4	Dodecane, 5-cyclohexyl-
1000406-32-4*	Dotriacontane, 1-iodo-
55333-99-8	Eicosane, 7-hexyl-
506-30-9	Eicosanoic acid
1000424-12-6*	Eicosanoic acid hexyl ester
103799-74-2	Elaidic acid lauryl ester
122-99-6	Ethanol, 2-phenoxy-
55591-10-1	Ethanone, 1-(2,3-dihydro-1,1-dimethyl-1H-inden-4-yl)-
6100-74-9	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-
34061-75-1	Ether, 3-butenyl propyl
97-53-0	Eugenol
110-17-8	Fumaric Acid



1000330-54-1*	Fumaric acid, ethyl 2-methylallyl ester
506-26-3	Gamolenic acid
102-62-5	Glycerol 1,2-diacetate
629-94-7	Heneicosane
630-04-6	Hentriacontane
72934-03-3	Heptacosanal
7194-84-5	Heptatriacontane
26627-85-0	Hexacosanal
111-06-8	Hexadecanoic acid, butyl ester
42232-25-7	Hexadecanoic acid, hexyl ester
2416-20-8	Hexadecenoic acid, Z-11-
149-57-5	Hexanoic acid, 2-ethyl-
123-31-9	Hydroquinone
857259	Isobutyl 4-hydroxybenzoate
121-91-5	Isophthalic acid
39702-28-8	Isopimara-9(11),15-diene
22882-95-7	Isopropyl linoleate
34424-57-2	Kaurene
37112-31-5	Levogluconone
506-21-8	Linoelaidic acid
1493515	Loliolide
4931-66-2	L-Proline, 5-oxo-, methyl ester
545-47-1	Lupeol
110-16-7	Maleic acid
6915-15-7	Malic Acid
118-71-8	Maltol
30364-38-6	Naphthalene, 1,2-dihydro-1,1,6-trimethyl-
511-02-4	Naphthalene, decahydro-1,1,4a-trimethyl-6-methylene-5-(3-methylene-4-pentenyl)-, [4aS-(4a.alpha.,5.alpha.,8a.beta.)]-
504-96-1	Neophytadiene
54773-06-7	N-Ethyl-2-isopropoxycarbonylazetidide
18835-35-3	Nonacos-1-ene
504-55-2	Nonacosan-10-ol
72934-04-4	Nonacosanal
630-03-5	Nonacosane
1000414-94-1*	Nonacosane-10,12-dione
58170-84-6	Nonacosane-8,10-dione
506-51-4	n-Tetracosanol-1
22725-64-0	Octacosanal
630-02-4	Octacosane
1560-98-1	Octacosane, 2-methyl-



557-61-9	Octacosanol
123-95-5	Octadecanoic acid, butyl ester
3460-37-5	Octadecanoic acid, hexyl ester
124-07-2	Octanoic acid
112-80-1	Oleic Acid
34900-26-0	Oxazole, 2-(8Z)-8-heptadecen-1-yl-4,5-dihydro-
7400-08-0	p-Coumaric acid
3973-22-6	p-Dioxin, 2,3-dihydro-5-methyl-
58196-28-4	Pentacosanal
629-99-2	Pentacosane
1002-84-2	Pentadecanoic acid
108906-10-1	Pentyl linoleate
120-95-6	Phenol, 2,4-bis(1,1-dimethylpropyl)-
6627-88-9	Phenol, 2,6-dimethoxy-4-(2-propenyl)-
15314	Phenol, 2-methoxy-3-(2-propenyl)-
644-35-9	Phenol, 2-propyl-
501-92-8	Phenol, 4-(2-propenyl)-
616-55-7	Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl-
28343-22-8	Phenol, 4-ethenyl-2,6-dimethoxy-
621-58-9	Phenol, 5-ethenyl-2-methoxy-
60-12-8	Phenylethyl Alcohol
85-44-9	Phthalic anhydride
1609-86-5	Propane, 2-isocyanato-2-methyl-
5654-86-4	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(2-methylpropyl)-
69-72-7	Salicylic acid
17963-04-1	Silane, [3-(2,3-epoxypropoxy)propyl]ethoxydimethyl-
2117-34-2	Silane, triethylmethoxy-
22635-78-5	Spiro[3.3]hepta-1,5-diene
4970-37-0	Stigmasta-3,5-diene
481-14-1	Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24Z)-
83-48-7	Stigmasterol
100-21-0	Terephthalic acid
57866-08-7	Tetracosanal
646-31-1	Tetracosane
557-59-5	Tetracosanoic acid
629-59-4	Tetradecane
21145-77-7	Tonalid
13474-59-4	trans-.alpha.-Bergamotene
1000405-19-1*	trans-9-Octadecenoic acid, pentyl ester
5932-68-3	trans-Isoeugenol
102-76-1	Triacetin



22725-63-9	Triacontanal
1000406-32-3*	Triacontane, 1-iodo-
39754-77-3	Tricosan-2-ol
638-67-5	Tricosane
629-50-5	Tridecane
13287-21-3	Tridecane, 6-methyl-
121-33-5	Vanillin
59-02-9	Vitamin E
1000130-89-5*	Z,Z-10,12-Hexadecadien-1-ol acetate
1000245-71-0*	Z-1,9-Dodecadiene

* Not official CAS Registry Numbers: “pseudo” identifiers created by NIST to link mass spectral records to corresponding chemical structures in the structure add-on files when an official CAS number was unavailable.

Table A4: List of chemicals tentatively identified in the yogurt package.

CAS number	Name
1000366-95-2*	(3E,6E)-Nona-3,6-dienyl 2-methylbutanoate
3047-32-3	(3-Ethyloxetan-3-yl)methanol
544-71-8	(9E,11E)-Octadecadienoic acid
20675-95-0	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol
6114-18-7	(E)-9-Octadecenoic acid ethyl ester
30689-78-2	(R)-(-)-(Z)-14-Methyl-8-hexadecen-1-ol
1000144-07-1*	(S)-3-Ethyl-4-methylpentanol
84060-80-0	(Z)-(Z)-Hex-3-en-1-yl 2-methylbut-2-enoate
71978-00-2	(Z)-5-Octenyl acetate
67883-79-8	(Z)-Hex-3-enyl (E)-2-methylbut-2-enoate
638-95-9	.alpha.-Amyrin
98-55-5	.alpha.-Terpineol
559-70-6	.beta.-Amyrin
495-61-4	.beta.-Bisabolene
713-95-1	.delta.-Dodecalactone
2305-05-7	.gamma.-Dodecalactone
83-47-6	.gamma.-Sitosterol
1000357-25-8*	1, 1,5-Trimethyl-1,2-dihydronaphthalene
112-47-0	1,10-Decanediol
5876-87-9	1,11-Dodecadiene
14722-40-8	1,15-Pentadecanediol
14811-95-1	1,19-Eicosadiene
1020-31-1	1,2-Benzenediol, 3,5-bis(1,1-dimethylethyl)-
1000329-72-1*	1,2-Benzenediol, O-(4-methoxybenzoyl)-O'-(2-furoyl)-
94-33-7	1,2-Ethanediol, monobenzoate



1129-92-6	1,3-Cyclododecadiene, (E,Z)-
40085-08-3	1,3-Cyclohexadiene, 5-ethyl-
77-99-6	1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-
24252-85-5	1,4,8-Dodecatriene, (E,E,E)-
6422-86-2	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester
1000221-85-9*	1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-
62338-27-6	1,5,9,11-Tridecatetraene, 12-methyl-, (E,E)-
16538-88-8	1,5-Cyclooctadiene, 3-(1-methyl-2-propenyl)-
295-63-6	1,6,11-Trioxacyclopentadecane
777-95-7	1,6-Dioxacyclododecane-7,12-dione
1686-30-2	1,7-Octadiene, 2-methyl-6-methylene-
80625-30-5	1,E-8,Z-10-Tridecatriene
83085-83-0	1,Z-5,E-7-Dodecatriene
56862-62-5	10-Methylnonadecane
2774-84-7	10-Undecyn-1-ol
6186-98-7	11-cis-Vaccenyl acetate
35289-31-7	11-Dodecenol
52380-33-3	11-Octadecenoic acid, methyl ester
75853-51-9	13-Methyltetradecanal
1000131-00-4*	13-Tetradecene-11-yn-1-ol
34450-18-5	17-Octadecynoic acid
7150-55-2	1-Butanone, 4-chloro-1-(4-hydroxyphenyl)-
21078-65-9	1-Decanol, 2-ethyl-
2425-77-6	1-Decanol, 2-hexyl-
45235-48-1	1-Decanol, 2-octyl-
110225-00-8	1-Dodecanol, 2-hexyl-
5333-42-6	1-Dodecanol, 2-octyl-
112-41-4	1-Dodecene
629-96-9	1-Eicosanol
15594-90-8	1-Heneicosanol
2004-39-9	1-Heptacosanol
6765-39-5	1-Heptadecene
26186-00-5	1-Heptadecyne
10042-59-8	1-Heptanol, 2-propyl-
1653-40-3	1-Heptanol, 6-methyl-
506-52-5	1-Hexacosanol
18835-33-1	1-Hexacosene
36653-82-4	1-Hexadecanol
1470-94-6	1H-Inden-5-ol, 2,3-dihydro-



237742-62-0	1-Methoxyoctacosane
18435-45-5	1-Nonadecene
112-92-5	1-Octadecanol
1000406-29-3*	1-Octadecanol, methyl ether
112-88-9	1-Octadecene
3913-02-8	1-Octanol, 2-butyl-
818-81-5	1-Octanol, 2-methyl-
765-13-9	1-Pentadecyne
74752-91-3	1-Tetradecen-3-yne
3133-01-5	1-Tricosanol
18835-32-0	1-Tricosene
2437-56-1	1-Tridecene
74630-39-0	1-Undecene, 4-methyl-
74630-42-5	1-Undecene, 7-methyl-
74630-40-3	1-Undecene, 8-methyl-
74630-41-4	1-Undecene, 9-methyl-
17312-44-6	2,3-Dimethyldecane
59920-26-2	2,4,6,8-Tetramethyl-1-undecene
54965-43-4	2,4-Cyclohexadien-1-one, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-
2363-88-4	2,4-Decadienal
96-76-4	2,4-Di-tert-butylphenol
719-22-2	2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-
13187-99-0	2-Bromo dodecane
23726-93-4	2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)-
939-55-9	2-Chloroethyl benzoate
1000357-24-9*	2-Cyclohexylnonadecane
58670-89-6	2-Decyl-1-tetradecanol
1653-37-8	2-Dodecanol, 2-methyl-
74744-37-9	2-Dodecen-4-yne, (Z)-
20407-84-5	2-Dodecenal, (E)-
118-60-5	2-Ethylhexyl salicylate
487-06-9	2H-1-Benzopyran-2-one, 5,7-dimethoxy-
2922-51-2	2-Heptadecanone
19780-79-1	2-Hexyl-1-octanol
7370-44-7	2H-Pyran-2-one, tetrahydro-6-undecyl-
7473-98-5	2-Hydroxy-iso-butyrophenone
7786-61-0	2-Methoxy-4-vinylphenol
1195-09-1	2-Methoxy-5-methylphenol
1010215-28-0*	2-Methylbicyclo[3.2.1]octane



1561-00-8	2-Methylheptacosane
1561-02-0	2-Methylhexacosane
27570-83-8	2-Methyltetradecan-2-ol
629-66-3	2-Nonadecanone
18829-56-6	2-Nonenal, (E)-
18479-57-7	2-Octanol, 2,6-dimethyl-
2345-28-0	2-Pentadecanone
502-69-2	2-Pentadecanone, 6,10,14-trimethyl-
195194-80-0	2-Piperidinone, N-[4-bromo-n-butyl]-
104-54-1	2-Propen-1-ol, 3-phenyl-
1653-31-2	2-Tridecanol
593-08-8	2-Tridecanone
10059-13-9	2-Undecanethiol, 2-methyl-
112-12-9	2-Undecanone
74630-45-8	2-Undecene, 9-methyl-, (Z)-
494-99-5	3,4-Dimethoxytoluene
1620-98-0	3,5-di-tert-Butyl-4-hydroxybenzaldehyde
928-80-3	3-Decanone
55499-02-0	3-Decene, 2,2-dimethyl-, (E)-
74685-33-9	3-Eicosene, (E)-
34303-81-6	3-Hexadecene, (Z)-
6702-50-7	3-Hydroxy-4-methoxybenzoic acid, methyl ester
81974-61-0	3-Methylbutyl hexadecanoate
20129-49-1	3-Methyldotriacontane
16626-48-5	3-Methylene-1,6-heptadiene
7206-19-1	3-Octadecene, (E)-
61886-64-4	3-Octadecyne
122-97-4	3-Phenylpropanol
74663-68-6	3-Tetradecen-5-yne, (Z)-
41446-68-8	3-Tetradecene, (E)-
74630-53-8	3-Undecene, 7-methyl-, (E)-
74630-49-2	3-Undecene, 7-methyl-, (Z)-
74630-50-5	3-Undecene, 9-methyl-, (Z)-
26931-99-7	4-Methoxy-3-(isopenten-2-yl)acetophenone
2277-16-9	4-Nonenal, (E)-
1010406-11-0*	4-Pentenoic acid, 2-methyl-, heptyl ester
41446-65-5	4-Tetradecene, (Z)-
74630-56-1	4-Undecene, 9-methyl-, (Z)-
1010360-41-7*	5,5-Diethylheptadecane



1117-52-8	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (E,E)-
3796-70-1	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-
3879-26-3	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-
51652-47-2	5-Decen-1-ol, (Z)-
16676-96-3	5-Dodecen-1-ol, acetate, (Z)-
7206-28-2	5-Dodecene, (Z)-
19780-12-2	5-Dodecyne
74685-30-6	5-Eicosene, (E)-
14300-89-1	5-Hydroxy-4,5-dimethyl-2,5-dihydrofuran-2-one
64275-73-6	5-Octen-1-ol, (Z)-
74630-67-4	5-Undecene, 3-methyl-, (E)-
97423-85-3	6,7-Diazabicyclo[3.2.2]non-6-ene, 2-methylene-
1215128-07-6	6-Methyl-4-heptenyl pentanoate
2777-58-4	6-Octadecenoic acid, methyl ester, (Z)-
22026-12-6	6-Tridecanone
82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione
82253-09-6	7-Propylidene-bicyclo[4.1.0]heptane
35216-11-6	7-Tetradecyne
19781-86-3	8-Hexadecyne
51760-35-1	9,11-Dodecadien-1-ol, acetate, (Z)-
463-40-1	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
1191-41-9	9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-
301-00-8	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-
60-33-3	9,12-Octadecadienoic acid (Z,Z)-
112-63-0	9,12-Octadecadienoic acid (Z,Z)-, methyl ester
1000352-65-1*	9-Decen-1-ol, methyl ether
17643-36-6	9-Decyn-1-ol
71899-38-2	9-Eicosyne
540-08-9	9-Heptadecanone
7206-25-9	9-Octadecene, (E)-
112-79-8	9-Octadecenoic acid, (E)-
2553-17-5	9-Oxononanoic acid
1000190-45-8*	Acetic acid, 3-acetoxy-1-(2-acetoxy-1-methyl-ethyl)-2-methyl-propyl ester
112-17-4	Acetic acid, decyl ester
84682-19-9	Acetic acid, methoxy-, 2-phenylethyl ester
112-14-1	Acetic acid, octyl ester
1000445-97-4*	Adipate Diethylene glycol cyclic dimer
498-02-2	Apocynin
661-19-8	Behenic alcohol



621-59-0	Benzaldehyde, 3-hydroxy-4-methoxy-
134-96-3	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-
104-87-0	Benzaldehyde, 4-methyl-
487-11-6	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-
108-70-3	Benzene, 1,3,5-trichloro-
1014-60-4	Benzene, 1,3-bis(1,1-dimethylethyl)-
6386-38-5	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester
2082-79-3	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester
496-16-2	Benzofuran, 2,3-dihydro-
65-85-0	Benzoic acid
1000375-33-4*	Benzoic acid, 2-(1-methylpropyl)oxy-, methyl ester
120-50-3	Benzoic acid, 2-methylpropyl ester
94-50-8	Benzoic acid, octyl ester
2049-96-9	Benzoic acid, pentyl ester
497-32-5	Bicyclo[2.2.1]heptane, 2,2-dimethyl-5-methylene-
89243-94-7	Bicyclo[3.2.0]heptane, 2-methylene-
1965-38-4	Bicyclo[3.2.1]octan-2-ol, exo-
26788-91-0	Bicyclo[3.2.2]nona-6,8-dien-3-one
54211-14-2	Bicyclo[4.1.0]heptane, 7-methylene-
41977-45-1	Bicyclo[4.1.0]heptane, 7-pentyl-
40954-37-8	Bicyclo[4.3.0]nonane, 2-methylene-, cis-
118-65-0	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4Z,9S*)]-
61142-73-2	Borinic acid, diethyl-, 1-cyclododecen-1-yl ester
626-11-9	Butanedioic acid, hydroxy-, diethyl ester, (.+/-.)-
39026-94-3	Butanoic acid, 1-methylhexyl ester
27625-35-0	Butanoic acid, 2-methyl-, 3-methylbutyl ester
625-08-1	Butanoic acid, 3-hydroxy-3-methyl-
140-26-1	Butanoic acid, 3-methyl-, 2-phenylethyl ester
659-70-1	Butanoic acid, 3-methyl-, 3-methylbutyl ester
56423-43-9	Butanoic acid, 3-methyl-, heptyl ester
10032-13-0	Butanoic acid, 3-methyl-, hexyl ester
7786-58-5	Butanoic acid, 3-methyl-, octyl ester
13562-84-0	Butanoic acid, 3-oxo-, hexyl ester
5454-09-1	Butanoic acid, decyl ester
2639-63-6	Butanoic acid, hexyl ester
110-39-4	Butanoic acid, octyl ester
1000336-54-6*	Butyl 9,12,15-octadecatrienoate



1000406-41-4*	Butyl tetratriacontyl ether
128-37-0	Butylated Hydroxytoluene
474-62-4	Campesterol
105-60-2	Caprolactam
1000383-25-7*	Carbonic acid, decyl vinyl ester
1000382-54-3*	Carbonic acid, eicosyl vinyl ester
1000383-25-6*	Carbonic acid, nonyl vinyl ester
1000382-54-4*	Carbonic acid, octadecyl vinyl ester
629-73-2	Cetene
80419-02-9	Chloromethyl 6-chlorododecanoate
474-77-1	Cholest-5-en-3-ol, (3.alpha.)-
747-90-0	Cholesta-3,5-diene
56797-43-4	cis,cis,cis-7,10,13-Hexadecatrienal
56829-23-3	cis,cis-7,10,-Hexadecadienal
13126-39-1	cis-13-Octadecenoic acid
53398-85-9	cis-3-Hexenyl-.alpha.-methylbutyrate
1000215-29-0*	cis-3-Methyl-endo-tricyclo[5.2.1.0(2.6)]decane
14959-86-5	cis-7-Dodecen-1-yl acetate
506-17-2	cis-Vaccenic acid
4651-54-1	Clionasterol acetate
1000253-25-3*	Cyclobutane-1,1-dicarboxamide, N,N'-di-benzoyloxy-
1502-05-2	Cyclodecanol
294-62-2	Cyclododecane
1129-90-4	Cyclododecyne
296-56-0	Cycloeicosane
295-65-8	Cyclohexadecane
74663-71-1	Cyclohexane, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-
61142-24-3	Cyclohexane, 1,2,4,5-tetraethyl-, (1.alpha.,2.alpha.,4.alpha.,5.alpha.)-
74742-35-1	Cyclohexane, 1,5-diethenyl-3-methyl-2-methylene-, (1.alpha.,3.alpha.,5.alpha.)-
16580-26-0	Cyclohexane, 1-isopropyl-1-methyl-
2114-42-3	Cyclohexane, 2-propenyl-
695-12-5	Cyclohexane, ethenyl-
4292-75-5	Cyclohexane, hexyl-
3282-53-9	Cyclohexene, 1-butyl-
766-03-0	Cyclohexene, 3-ethenyl-
586-67-4	Cyclohexene, 4-methyl-1-(1-methylethenyl)-
3964-66-7	Cyclohexene,1-hexyl-
15232-78-7	Cyclohexene,3-hexyl-
2213-60-7	Cyclooctene, 3-ethenyl-



1000156-73-8*	Cyclopentane, 1-hydroxymethyl-1,3-dimethyl-
62199-51-3	Cyclopentane, 1-pentyl-2-propyl-
6703-82-8	Cyclopentane, heneicosyl-
2882-98-6	Cyclopentane, nonyl-
6785-23-5	Cyclopentane, undecyl-
4028-59-5	Cyclopentanol, 1,2-dimethyl-3-(1-methylethenyl)-, [1R-(1.alpha.,2.alpha.,3.beta.)]-
61142-66-3	Cyclopentene, 5-hexyl-3,3-dimethyl-
22822-99-7	Cyclopropane, 1-ethenyl-2-hexenyl-, [1.alpha.,2.beta.(E)]-(./-.)-
1472-09-9	Cyclopropane, octyl-
297-03-0	Cyclotetracosane
295-17-0	Cyclotetradecane
295-02-3	Cyclotridecane
62338-14-1	Decane, 3,3,6-trimethyl-
75029-95-7	Decane, 5-methyl-6-methylene-
110-38-3	Decanoic acid, ethyl ester
20777-49-5	Dihydrocarvyl acetate
753-70-8	Dimethylphosphinic fluoride
55401-55-3	Docosane, 11-decyl-
1000406-37-9*	Docosyl nonyl ether
112-40-3	Dodecane
143-07-7	Dodecanoic acid
106-33-2	Dodecanoic acid, ethyl ester
1000406-32-4*	Dotriacontane, 1-iodo-
1000351-84-2*	Dotriacontyl heptafluorobutyrate
1010406-33-6*	Dotriacontyl isobutyl ether
16695-41-3	E-7-Dodecen-1-ol acetate
1000130-92-0*	E-7-Octadecene
54833-23-7	Eicosane, 10-methyl-
55333-99-8	Eicosane, 7-hexyl-
4443-61-2	Eicosane, 9-cyclohexyl-
1000513-01-3*	Epilupeol; 20(29)-Lupen-3alpha-ol (isomer 1)
474-63-5	Ergosta-5,24(28)-dien-3-ol, (3.beta.)-
122-99-6	Ethanol, 2-phenoxy-
6100-74-9	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-
4610-69-9	Ethyl (Z)-cinnamate
1113-92-4	Ethylmalonic acid dibutyl ester
97-53-0	Eugenol
1000367-88-7*	Formic acid, 3-phenylpropyl ester
17605-67-3	Fucosterol



593-85-1	Guanidine carbonate
55282-11-6	Heneicosane, 11-(1-ethylpropyl)-
1000351-83-8*	Heneicosyl heptafluorobutyrate
1000351-76-5*	Heneicosyl trifluoroacetate
630-04-6	Hentriacontane
593-49-7	Heptacosane
61868-03-9	Heptadecane, 2,3-dimethyl-
26429-11-8	Heptadecane, 4-methyl-
7225-64-1	Heptadecane, 9-octyl-
506-12-7	Heptadecanoic acid
7194-84-5	Heptatriacontane
1000406-40-0*	Heptyl octacosyl ether
1000406-40-1*	Heptyl triacontyl ether
55429-83-9	Hexacosane, 9-octyl-
1000351-83-3*	Hexacosyl heptafluorobutyrate
629-80-1	Hexadecanal
110-34-9	Hexadecanoic acid, 2-methylpropyl ester
111-06-8	Hexadecanoic acid, butyl ester
628-97-7	Hexadecanoic acid, ethyl ester
112-39-0	Hexadecanoic acid, methyl ester
2416-20-8	Hexadecenoic acid, Z-11-
1000406-38-6*	Hexadecyl octyl ether
1000351-89-0*	Hexatriacontyl pentafluoropropionate
17071-54-4	Hexyl octyl ether
29812-79-1	Hydroxylamine, O-decyl-
7779-65-9	Isoamyl cinnamate
37811-72-6	Isobutyl laurate
1000406-33-5*	Isobutyl triacontyl ether
2198-61-0	Isopentyl hexanoate
505-32-8	Isophytol
1000433-23-4*	Isovaleric acid, decyl ester
544-35-4	Linoleic acid ethyl ester
947-19-3	Methanone, (1-hydroxycyclohexyl)phenyl-
1000336-35-1*	Methyl 8,11,14-heptadecatrienoate
13058-52-1	Methyl 9-cis,11-trans-octadecadienoate
1000406-30-1*	Methyl tetratriacontyl ether
1000406-29-9*	Methyl triacontyl ether
93-15-2	Methyleugenol
53156-11-9	Naphthalene, 1,2-dihydro-4,5,7-trimethyl-



91-57-6	Naphthalene, 2-methyl-
334-48-5	n-Decanoic acid
1454-84-8	n-Nonadecanol-1
18835-35-3	Nonacos-1-ene
630-03-5	Nonacosane
14167-67-0	Nonacosane, 3-methyl-
124-19-6	Nonanal
7323-15-1	Nonane, 2,8-dimethyl-4-methylene-
112-05-0	Nonanoic acid
57943-67-6	Nonanoic acid, 2-phenylethyl ester
1000406-38-2*	Nonyl octacosyl ether
1000406-38-0*	Nonyl tetracosyl ether
506-51-4	n-Tetracosanol-1
630-02-4	Octacosane
1560-98-1	Octacosane, 2-methyl-
557-61-9	Octacosanol
1010351-83-6*	Octacosyl heptafluorobutyrate
1000351-74-9*	Octacosyl trifluoroacetate
638-66-4	Octadecanal
593-45-3	Octadecane
57-11-4	Octadecanoic acid
111-61-5	Octadecanoic acid, ethyl ester
79392-43-1	Octadecyl trifluoroacetate
1000543-48-2*	Octahydro-2H-indeno[1,2-b:5,6-b']bis(oxirene) (isomer 2)
62016-37-9	Octane, 2,4,6-trimethyl-
124-07-2	Octanoic acid
1000280-56-1*	Octanoic acid, undec-10-enyl ester
33580-04-0	Octatriene, 1,3-trans-5-trans-
6197-30-4	Octocrylene
112-80-1	Oleic Acid
123-69-3	Oxacycloheptadec-8-en-2-one, (8Z)-
1000309-24-0*	Oxalic acid, allyl dodecyl ester
1000309-24-4*	Oxalic acid, allyl hexadecyl ester
1000309-24-2*	Oxalic acid, allyl tetradecyl ester
3497-06-1	Oxirane, 2-[(decyloxy)methyl]-
1000307-63-9*	p-Anisic acid, 4-nitrophenyl ester
629-99-2	Pentacosane
3892-00-0	Pentadecane, 2,6,10-trimethyl-
52997-43-0	Pentadecane, 7-(bromomethyl)-



1002-84-2	Pentadecanoic acid
2306-91-4	Pentadecanoic acid, 3-methylbutyl ester
5549-09-7	Pentalene, 1,2,3,3a,4,6a-hexahydro-
1755-05-1	Pentalene, octahydro-, cis-
54889-47-3	Pentane, 2,2'-[ethylidenebis(oxy)]bis-
630-07-9	Pentatriacontane
55255-56-6	Phenanthrene, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl-
31570-04-4	Phenol, 2,4-bis(1,1-dimethylethyl)-, phosphite (3:1)
6627-88-9	Phenol, 2,6-dimethoxy-4-(2-propenyl)-
5912-86-7	Phenol, 2-methoxy-4-(1-propenyl)-, (Z)-
80-46-6	Phenol, 4-(1,1-dimethylpropyl)-
28343-22-8	Phenol, 4-ethenyl-2,6-dimethoxy-
645-56-7	Phenol, 4-propyl-
621-58-9	Phenol, 5-ethenyl-2-methoxy-
60-12-8	Phenylethyl Alcohol
1000315-48-0*	Phthalic acid, octyl 2-pentyl ester
150-86-7	Phytol
103-48-0	Propanoic acid, 2-methyl-, 2-phenylethyl ester
103-58-2	Propanoic acid, 2-methyl-, 3-phenylpropyl ester
5454-19-3	Propanoic acid, decyl ester
62238-24-8	Spiro[2.4]heptane, 1,5-dimethyl-6-methylene-
185-65-9	Spiro[2.5]octane
121080-73-7	Spiro[cyclopropane-1,2'-[6.7]diazabicyclo[3.2.2]non-6-ene]
111-02-4	Squalene
20290-75-9	Stearidonic acid
481-14-1	Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24Z)-
7212-91-1	Stigmasta-7,24(28)-dien-3-ol, (3.beta.,5.alpha.)-
83-48-7	Stigmasterol
1000309-12-4*	Sulfurous acid, 2-propyl tridecyl ester
1000309-18-4*	Sulfurous acid, butyl heptadecyl ester
1010309-13-6*	Sulfurous acid, hexyl tetradecyl ester
1000309-13-3*	Sulfurous acid, hexyl undecyl ester
1000309-12-7*	Sulfurous acid, octadecyl 2-propyl ester
1000309-14-4*	Sulfurous acid, pentyl undecyl ester
55429-84-0	Tetracosane, 11-decyl-
1000351-83-7*	Tetracosyl heptafluorobutyrate
1000487-16-3*	Tetracyclo[5.4.0.0(3,5).0(8,10)]undecane (exo,endo-isomer)
629-59-4	Tetradecane
55045-14-2	Tetradecane, 4-ethyl-



544-63-8	Tetradecanoic acid
134896-10-9	Tetradecatriene,3Z,6Z,9Z-
1000351-84-1*	Tetratriacontyl heptafluorobutyrate
1000351-81-5*	Tetratriacontyl pentafluoropropionate
108-88-3	Toluene
21145-77-7	Tonalid
22057-21-2	trans,trans-2,9-Undecadiene
1000333-61-3*	trans-13-Octadecenoic acid, methyl ester
1000364-13-3*	trans-2-Methylcyclohexanol, trifluoroacetate
1000364-13-8*	trans-4-Methylcyclohexanol, trifluoroacetate
18383-58-9	trans-Chrysanthemol
638-68-6	Triacontane
1000406-32-3*	Triacontane, 1-iodo-
1000351-83-2*	Triacontyl heptafluorobutyrate
1928-30-9	Tricosane, 2-methyl-
1000351-83-4*	Tricosyl heptafluorobutyrate
1000351-75-1*	Tricosyl trifluoroacetate
1000190-80-8*	Tricyclo[5.2.1.0(1,5)]decane
53130-27-1	Tricyclo[5.3.0.0(3,9)]decane
26730-12-1	Tridecane, 4-methyl-
19780-80-4	Tridecane, 7-methylene-
2665-11-4	Trihexadecyl borate
17312-77-5	Undecane, 2,3-dimethyl-
5698-48-6	Undecane, 5-methylene-
121-33-5	Vanillin
59-02-9	Vitamin E
13857-03-9	Z-7-Decen-1-yl acetate

* Not official CAS Registry Numbers: “pseudo” identifiers created by NIST to link mass spectral records to corresponding chemical structures in the structure add-on files when an official CAS number was unavailable.

Table A5: List of chemicals tentatively identified in the yogurt foodstuff

CAS number	Name
544-71-8	(9E,11E)-Octadecadienoic acid
20675-95-0	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl)phenol
6114-18-7	(E)-9-Octadecenoic acid ethyl ester
64566-18-3	(R)-(-)-14-Methyl-8-hexadecyn-1-ol
110453-78-6	(S)-(+)-6-Methyl-1-octanol
77899-11-7	(Z)6,(Z)9-Pentadecadien-1-ol
638-95-9	.alpha.-Amyrin
498-36-2	.alpha.-Hydroxyisocaproic acid



58-95-7	.alpha.-Tocopheryl acetate
559-70-6	.beta.-Amyrin
498-07-7	.beta.-D-Glucopyranose, 1,6-anhydro-
17289-61-1	.beta.-D-Ribopyranoside, methyl
148-03-8	.beta.-Tocopherol
3301-94-8	.delta.-Nonalactone
83-47-6	.gamma.-Sitosterol
5876-87-9	1,11-Dodecadiene
21964-49-8	1,13-Tetradecadiene
14722-40-8	1,15-Pentadecanediol
80-09-1	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester
107-88-0	1,3-Butanediol
24252-85-5	1,4,8-Dodecatriene, (E,E,E)-
62338-27-6	1,5,9,11-Tridecatetraene, 12-methyl-, (E,E)-
295-63-6	1,6,11-Trioxacyclopentadecane
50871-05-1	1,6-Heptadiene, 3-methyl-
62108-28-5	1,7-Nonadiene, 4,8-dimethyl-
10482-53-8	1,8,11,14-Heptadecatetraene, (Z,Z,Z)-
56134-03-3	1,8,11-Heptadecatriene, (Z,Z)-
1000436-69-3*	1,9-Cyclohexadecadiene (isomer 3)
80625-36-1	1,E-11,Z-13-Octadecatriene
2420-56-6	10E,12Z-Octadecadienoic acid
112-45-8	10-Undecenal
2774-84-7	10-Undecyn-1-ol
2463-02-7	11,14-Eicosadienoic acid, methyl ester
56683-54-6	11-Hexadecen-1-ol, (Z)-
65686-49-9	11-Hexadecyn-1-ol
58594-45-9	13-Octadecenal, (Z)-
286-99-7	13-Oxabicyclo[10.1.0]tridecane
1000131-00-4*	13-Tetradecene-11-yn-1-ol
34450-18-5	17-Octadecynoic acid
4426-47-5	1-Butaneboronic acid
7150-55-2	1-Butanone, 4-chloro-1-(4-hydroxyphenyl)-
114614-83-4	1-Cyclohexylheptene
2425-77-6	1-Decanol, 2-hexyl-
13942-77-3	1-Deoxy-d-arabitol
629-96-9	1-Eicosanol
16681-68-8	1H-1,2,3-Triazole-4-carboxaldehyde
18835-33-1	1-Hexacosene



36653-82-4	1-Hexadecanol
629-74-3	1-Hexadecyne
4843-98-5	1H-pyrazol-4-ol
26964-49-8	1H-Pyrazole, 4,5-dihydro-3-methyl-1-propyl-
20845-34-5	1-Methyl-2-piperidinemethanol
1000522-25-6*	1-Methyl-4-(4-methylpent-3-en-1-yl)cyclohex-3-enecarbaldehyde (isomer 2)
55195-08-9	1-Methylbutyl hexadecanoate
4601-85-8	1-Methyltricyclo[2.2.1.0(2,6)]heptane
18435-45-5	1-Nonadecene
35192-73-5	1-Nonen-4-ol
629-89-0	1-Octadecyne
765-13-9	1-Pentadecyne
75-84-3	1-Propanol, 2,2-dimethyl-
3054-95-3	1-Propene, 3,3-diethoxy-
10192-32-2	1-Tetracosene
1120-36-1	1-Tetradecene
765-10-6	1-Tetradecyne
18835-32-0	1-Tricosene
26186-02-7	1-Tridecyne
112-42-5	1-Undecanol
74744-28-8	1-Undecen-3-yne
2243-98-3	1-Undecyne
220556-75-2	2-((8Z,11Z)-Heptadeca-8,11-dien-1-yl)-4,5-dihydrooxazole
6846-50-0	2,2,4-Trimethyl-1,3-pentanediol diisobutyrate
71312-54-4	2,3-Diazabicyclo[2.2.1]hept-2-ene, 1,4-dimethyl-
1010458-45-6	2,3-dihydroxypropyl isobutyrate
51174-12-0	2,4,4-Trimethyl-1-hexene
2363-88-4	2,4-Decadienal
25152-84-5	2,4-Decadienal, (E,E)-
25152-83-4	2,4-Decadienal, (E,Z)-
96-76-4	2,4-Di-tert-butylphenol
7757-96-2	2,5-Furandione, dihydro-3-(1-octenyl)-
15233-65-5	2,6-Dimethoxyhydroquinone
94120-00-0	2-{2-[2-(Acryloyloxy)-1-methylethoxy]-1-methylethoxy}-1-methylethyl acrylate
7494-34-0	26-Nor-5-cholesten-3.beta.-ol-25-one
3913-81-3	2-Decenal, (E)-
2497-25-8	2-Decenal, (Z)-
4117-14-0	2-Decyn-1-ol



74744-38-0	2-Dodecen-4-yne, (E)-
74744-37-9	2-Dodecen-4-yne, (Z)-
1721-51-3	2H-1-Benzopyran-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyl-3,7,11-tridecatrienyl)-
22589-04-4	2-Heneicosanone
19776-81-9	2H-Pyran-2-carboxylic acid, 5-ethylidene-5,6-dihydro-2,3-dimethyl-6-oxo-, [S-(E)]-
100-72-1	2H-Pyran-2-methanol, tetrahydro-
2034-61-9	2-Hydroxy-1-(4-hydroxy-3-methoxyphenyl)-1-propanone
13436-45-8	2-Methoxytetrahydrofuran
1010215-28-0*	2-Methylbicyclo[3.2.1]octane
1468-39-9	2-Methylbutanoic anhydride
1561-02-0	2-Methylhexacosane
1560-78-7	2-Methyltetracosane
18829-56-6	2-Nonenal, (E)-
2345-28-0	2-Pentadecanone
2834-00-6	2-Pentadecyn-1-ol
56052-85-8	2-Pentene, 5-(pentyloxy)-, (E)-
1135-24-6	2-Propenoic acid, 3-(4-hydroxy-3-methoxyphenyl)-
621-82-9	2-Propenoic acid, 3-phenyl-
14293-08-4	2-Pyrrolidinone, 5-(cyclohexylmethyl)-
55194-58-6	2-Undecanol palmitate
112-12-9	2-Undecanone
2463-77-6	2-Undecenal
53448-07-0	2-Undecenal, E-
3142-58-3	3,3-Dimethyl-2,4-pentane dione
5803-57-6	3,4-Dihydroxy-5-methyl-dihydrofuran-2-one
29279-99-0	3,4-Dimethyl-5-hydroxy-isoxazole
4358-64-9	3,4-Furandiol, tetrahydro-, cis-
22554-74-1	3,4-Furandiol, tetrahydro-, trans-
59643-68-4	3,5-Dimethyl-3-heptene
102608-53-7	3,7,11,15-Tetramethyl-2-hexadecen-1-ol
1000144-12-7*	3,7,11-Trimethyl-3-hydroxy-6,10-dodecadien-1-yl acetate
74744-55-1	3-Heptadecen-5-yne, (Z)-
140235-34-3	3-Hydroxy-4-methoxy-4-oxobutanoic acid
645-08-9	3-Hydroxy-4-methoxybenzoic acid
62488-24-8	3-Methylbutyl tetradecanoate
4124-88-3	3-Nonenoic acid
61886-64-4	3-Octadecyne
1569-50-2	3-Penten-2-ol



74663-68-6	3-Tetradecen-5-yne, (Z)-
55182-74-6	3-Tetradecyn-1-ol
60186-78-9	3-Tridecene
5754-34-7	4-(2-Hydroxyethyl)-2,2-dimethyl-1,3-dioxolane
1000548-84-6*	4-Cycloocten-1-ol, trifluoroacetate
107289-20-3	4H-1,3-Dioxin-4-one, 2-(1,1-dimethylethyl)-6-methyl-, (R)-
28564-83-2	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-
1073-96-7	4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-
501-30-4	4H-Pyran-4-one, 5-hydroxy-2-(hydroxymethyl)-
2277-16-9	4-Nonenal, (E)-
1453-82-3	4-Pyridinecarboxamide
6053-02-7	4-Vinylbenzene-1,2-diol
1000531-26-2*	5-(1-Hydroxyethyl)oxolan-2-one (isomer 1)
1000531-26-3*	5-(1-Hydroxyethyl)oxolan-2-one (isomer 2)
1117-52-8	5,9,13-Pentadecatrien-2-one, 6,10,14-trimethyl-, (E,E)-
3796-70-1	5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-
3879-26-3	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-
67-47-0	5-Hydroxymethylfurfural
7212-53-5	5-Methyl-1-heptanol
4055-72-5	6-Hydroxyeugenol
1215128-07-6	6-Methyl-4-heptenyl pentanoate
80648-29-9	6-Methyloctahydrocoumarin
2777-58-4	6-Octadecenoic acid, methyl ester, (Z)-
1117-61-9	6-Octen-1-ol, 3,7-dimethyl-, (R)-
7561-64-0	7,10,13-Hexadecatrienoic acid, (Z,Z,Z)-
82304-66-3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione
96-08-2	7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(2-methyloxiranyl)-
82253-09-6	7-Propylidene-bicyclo[4.1.0]heptane
2579-04-6	8-Heptadecene
1000211-14-3*	8-Methylene-3-oxatricyclo[5.2.0.0(2,4)]nonane
1000452-08-1*	9(E),11(E)-Conjugated linoleic acid, ethyl ester
1000142-35-1*	9,10-Diazatricyclo[4.4.0.0(2,8)]dec-9-ene
463-40-1	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
1191-41-9	9,12,15-Octadecatrienoic acid, ethyl ester, (Z,Z,Z)-
301-00-8	9,12,15-Octadecatrienoic acid, methyl ester, (Z,Z,Z)-
506-43-4	9,12-Octadecadien-1-ol, (Z,Z)-
2277-28-3	9,12-Octadecadienoic acid (Z,Z)-, 2,3-dihydroxypropyl ester
112-63-0	9,12-Octadecadienoic acid (Z,Z)-, methyl ester
2462-85-3	9,12-Octadecadienoic acid, methyl ester



2566-97-4	9,12-Octadecadienoic acid, methyl ester, (E,E)-
7459-33-8	9,12-Octadecadienoyl chloride, (Z,Z)-
56554-35-9	9,17-Octadecadienal, (Z)-
1000503-97-9*	9,19-Cyclolanost-25-ene-3,24-diol
39770-05-3	9-Decenal
17643-36-6	9-Decyn-1-ol
71084-08-7	9-Dodecyn-1-ol
25107-01-1	9-Methylbicyclo[3.3.1]nonane
142-57-4	9-Octadecenoic acid (Z)-, pentyl ester
1937-62-8	9-Octadecenoic acid, methyl ester, (E)-
35365-59-4	9-Octadecyne
2553-17-5	9-Oxononanoic acid
27519-02-4	9-Tricosene, (Z)-
1000190-45-8*	Acetic acid, 3-acetoxy-1-(2-acetoxy-1-methyl-ethyl)-2-methyl-propyl ester
99-93-4	Acetophenone, 4'-hydroxy-
1000353-62-3*	Adipic acid, butyl 3-hexyl ester
498-02-2	Apocynin
15764-16-6	Benzaldehyde, 2,4-dimethyl-
621-59-0	Benzaldehyde, 3-hydroxy-4-methoxy-
123-08-0	Benzaldehyde, 4-hydroxy-
134-96-3	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-
80-07-9	Benzene, 1,1'-sulfonylbis[4-chloro-
487-11-6	Benzene, 1,2,3-trimethoxy-5-(2-propenyl)-
1014-60-4	Benzene, 1,3-bis(1,1-dimethylethyl)-
103-82-2	Benzeneacetic acid
104-53-0	Benzenepropanal
65-85-0	Benzoic acid
50-30-6	Benzoic acid, 2,6-dichloro-
23676-09-7	Benzoic acid, 4-ethoxy-, ethyl ester
99-96-7	Benzoic acid, 4-hydroxy-
530-57-4	Benzoic acid, 4-hydroxy-3,5-dimethoxy-
1010340-22-6*	Benzoic acid, tridecyl ester
13159-28-9	Betulinaldehyde
54766-91-5	Bicyclo[10.1.0]tridec-1-ene
17065-18-8	Bicyclo[2.1.0]pentane, 1,4-dimethyl-
497-32-5	Bicyclo[2.2.1]heptane, 2,2-dimethyl-5-methylene-
15185-11-2	Bicyclo[2.2.1]heptane, 2-methyl-
16189-46-1	Bicyclo[5.3.0]decane (cis)



118-65-0	Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-, [1R-(1R*,4Z,9S*)]-
110-15-6	Butanedioic acid
97-67-6	Butanedioic acid, hydroxy-, (S)-
107-90-4	Butanimidamide
4026-18-0	Butanoic acid, 2-hydroxy-3-methyl-
37064-20-3	Butanoic acid, 2-methyl-, propyl ester
2051-78-7	Butanoic acid, 2-propenyl ester
659-70-1	Butanoic acid, 3-methyl-, 3-methylbutyl ester
10032-13-0	Butanoic acid, 3-methyl-, hexyl ester
105-66-8	Butanoic acid, propyl ester
1000336-54-6*	Butyl 9,12,15-octadecatrienoate
128-37-0	Butylated Hydroxytoluene
474-62-4	Campesterol
105-60-2	Caprolactam
1000382-54-3*	Carbonic acid, eicosyl vinyl ester
1000382-90-2*	Carbonic acid, heptadecyl prop-1-en-2-yl ester
1000383-11-5*	Carbonic acid, octadecyl prop-1-en-2-yl ester
474-77-1	Cholest-5-en-3-ol, (3.alpha.)-
13126-39-1	cis-13-Octadecenoic acid
1000215-29-0*	cis-3-Methyl-endo-tricyclo[5.2.1.0(2.6)]decane
52207-99-5	cis-7,cis-11-Hexadecadien-1-yl acetate
2416-19-5	cis-7-Hexadecenoic acid
1000215-29-3*	Cis-8-methyl-exo-tricyclo[5.2.1.0(2.6)]decane
506-17-2	cis-Vaccenic acid
97-89-2	Citronellyl isobutyrate
1892-12-2	Cyclododecanemethanol
1129-90-4	Cyclododecyne
1003-64-1	Cyclohexane, ethylidene-
4516-69-2	Cyclopentane, 1,1,3-trimethyl-
32281-85-9	Cyclopentane, 2-isopropyl-1,3-dimethyl-
1472-09-9	Cyclopropane, octyl-
5336-08-3	D-(+)-Ribonic acid .gamma.-lactone
124-18-5	Decane
62108-22-9	Decane, 2,5,9-trimethyl-
62108-21-8	Decane, 6-ethyl-2-methyl-
20736-25-8	Dihydrosyringenin
10191-41-0	dl-.alpha.-Tocopherol
149-87-1	DL-Proline, 5-oxo-
1000406-31-9*	Docosane, 1-iodo-



4292-19-7	Dodecane, 1-iodo-
31295-56-4	Dodecane, 2,6,11-trimethyl-
1560-97-0	Dodecane, 2-methyl-
143-07-7	Dodecanoic acid
1000245-48-4*	E-10-Pentadecenol
1000406-31-8*	Eicosane, 1-iodo-
506-30-9	Eicosanoic acid
1000513-01-3*	Epilupeol; 20(29)-Lupen-3 α -ol (isomer 1)
474-63-5	Ergosta-5,24(28)-dien-3-ol, (3. β .)-
122-99-6	Ethanol, 2-phenoxy-
1450-72-2	Ethanone, 1-(2-hydroxy-5-methylphenyl)-
6100-74-9	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-
19467-01-7	Ethyl .alpha.-d-glucopyranoside
111-62-6	Ethyl Oleate
97-53-0	Eugenol
110-17-8	Fumaric Acid
629-94-7	Heneicosane
630-04-6	Hentriacontane
593-49-7	Heptacosane
506-12-7	Heptadecanoic acid
1000406-39-8*	Heptyl tetracosyl ether
26627-85-0	Hexacosanal
630-01-3	Hexacosane
110-34-9	Hexadecanoic acid, 2-methylpropyl ester
111-06-8	Hexadecanoic acid, butyl ester
628-97-7	Hexadecanoic acid, ethyl ester
42232-25-7	Hexadecanoic acid, hexyl ester
112-39-0	Hexadecanoic acid, methyl ester
1000405-18-9*	Hexadecanoic acid, pentyl ester
2416-20-8	Hexadecenoic acid, Z-11-
3658-93-3	Hexane, 1,1-diethoxy-
563-16-6	Hexane, 3,3-dimethyl-
30563-33-8	Hexanoic acid, 4-pentenyl ester
306-08-1	Homovanillic acid
501-52-0	Hydrocinnamic acid
5146-52-1	Imidazole, 2-methylamino-
110-27-0	Isopropyl myristate
506-21-8	Linoelaidic acid
544-35-4	Linoleic acid ethyl ester



98-79-3	L-Pyroglutamic acid
545-47-1	Lupeol
6915-15-7	Malic Acid
118-71-8	Maltol
947-19-3	Methanone, (1-hydroxycyclohexyl)phenyl-
13058-52-1	Methyl 9-cis,11-trans-octadecadienoate
112-61-8	Methyl stearate
511-02-4	Naphthalene, decahydro-1,1,4a-trimethyl-6-methylene-5-(3-methylene-4-pentenyl)-, [4aS-(4a.alpha.,5.alpha.,8a.beta.)]-
334-48-5	n-Decanoic acid
504-96-1	Neophytadiene
54773-06-7	N-Ethyl-2-isopropoxycarbonylazetidine
98-92-0	Niacinamide
18835-35-3	Nonacos-1-ene
72934-04-4	Nonacosanal
630-03-5	Nonacosane
1000414-94-1*	Nonacosane-10,12-dione
629-92-5	Nonadecane
17302-32-8	Nonane, 3,7-dimethyl-
1000239-48-8*	N-tert-Butylhydroxylamine
506-51-4	n-Tetracosanol-1
22725-64-0	Octacosanal
630-02-4	Octacosane
1560-98-1	Octacosane, 2-methyl-
557-61-9	Octacosanol
629-93-6	Octadecane, 1-iodo-
57-11-4	Octadecanoic acid
627-88-3	Octadecanoic acid, 3-methylbutyl ester
111-61-5	Octadecanoic acid, ethyl ester
1072-16-8	Octane, 2,7-dimethyl-
124-07-2	Octanoic acid
123-69-3	Oxacycloheptadec-8-en-2-one, (8Z)-
74685-36-2	Oxacyclotetradecane-2,11-dione, 13-methyl-
34900-26-0	Oxazole, 2-(8Z)-8-heptadecen-1-yl-4,5-dihydro-
85721-25-1	Oxirane, (7-octenyl)-
3234-28-4	Oxirane, dodecyl-
373-49-9	Palmitoleic acid
94134-03-9	Pearlate
16980-85-1	Pentacos-1-ene
629-99-2	Pentacosane



2765-11-9	Pentadecanal-
1002-84-2	Pentadecanoic acid
54889-47-3	Pentane, 2,2'-[ethylidenebis(oxy)]bis-
1000159-93-4*	Pentanoic acid, 10-undecenyl ester
488-15-3	Pentanoic acid, 2-hydroxy-3-methyl-
13748-90-8	Pentanoic acid, 2-hydroxy-4-methyl-, (S)-
2050-09-1	Pentanoic acid, 3-methylbutyl ester
108906-10-1	Pentyl linoleate
55255-56-6	Phenanthrene, 7-ethenyl-1,2,3,4,4a,5,6,7,8,9,10,10a-dodecahydro-1,1,4a,7-tetramethyl-
6627-88-9	Phenol, 2,6-dimethoxy-4-(2-propenyl)-
61499-22-7	Phenol, 4-(2-propenyl)-, acetate
60-12-8	Phenylethyl Alcohol
1000315-17-4*	Phthalic acid, 6-ethyl-3-octyl butyl ester
1000377-72-3*	Phthalic acid, di(oct-3-yl) ester
150-86-7	Phytol
1609-86-5	Propane, 2-isocyanato-2-methyl-
97-62-1	Propanoic acid, 2-methyl-, ethyl ester
644-49-5	Propanoic acid, 2-methyl-, propyl ester
69-72-7	Salicylic acid
62238-24-8	Spiro[2.4]heptane, 1,5-dimethyl-6-methylene-
20290-75-9	Stearidonic acid
521-03-9	Stigmast-7-en-3-ol, (3.beta.,5.alpha.)-
481-14-1	Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24Z)-
7212-91-1	Stigmasta-7,24(28)-dien-3-ol, (3.beta.,5.alpha.)-
83-48-7	Stigmasterol
1000309-20-2*	Sulfurous acid, 2-ethylhexyl hexyl ester
1000309-18-4*	Sulfurous acid, butyl heptadecyl ester
57866-08-7	Tetracosanal
646-31-1	Tetracosane
544-63-8	Tetradecanoic acid
1000405-19-1*	trans-9-Octadecenoic acid, pentyl ester
22725-63-9	Triacontanal
13287-21-3	Tridecane, 6-methyl-
1010115-66-1*	Tridecanol, 2-ethyl-2-methyl-
17301-30-3	Undecane, 3,8-dimethyl-
59-02-9	Vitamin E
51607-94-4	Z,E-7,11-Hexadecadien-1-yl acetate
1000130-89-5*	Z,Z-10,12-Hexadecadien-1-ol acetate



* Not official CAS Registry Numbers: “pseudo” identifiers created by NIST to link mass spectral records to corresponding chemical structures in the structure add-on files when an official CAS number was unavailable.

Table A6: List of chemicals tentatively identified in both packaging and foodstuff of both products

CAS	Name
1002-84-2	Pentadecanoic acid
112-12-9	2-Undecanone
122-99-6	Ethanol, 2-phenoxy-
124-07-2	Octanoic acid
1560-98-1	Octacosane, 2-methyl-
18435-45-5	1-Nonadecene
18835-32-0	1-Tricosene
18835-35-3	Nonacos-1-ene
2277-16-9	4-Nonenal, (E)-
2363-88-4	2,4-Decadienal
2777-58-4	6-Octadecenoic acid, methyl ester, (Z)-
3879-26-3	5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-
463-40-1	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-
474-62-4	Campesterol
481-14-1	Stigmasta-5,24(28)-dien-3-ol, (3.beta.,24Z)-
506-51-4	n-Tetracosanol-1
544-71-8	(9E,11E)-Octadecadienoic acid
557-61-9	Octacosanol
559-70-6	.beta.-Amyrin
59-02-9	Vitamin E
629-96-9	1-Eicosanol
629-99-2	Pentacosane
630-02-4	Octacosane
630-03-5	Nonacosane
630-04-6	Hentriacontane
638-95-9	.alpha.-Amyrin



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83-47-6	.gamma.-Sitosterol
83-48-7	Stigmasterol
97-53-0	Eugenol