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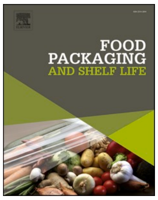

Exploring soda contamination coming from paper straws through ultra-high-pressure liquid chromatography coupled with an ion mobility-quadrupole time-of-flight analyzer and advanced statistical analysis

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ABSTRACT

This study deals with the migration of compounds from printed straws into a carbonated drink (soda), employing an innovative approach that combines Ultra-High-Pressure Liquid Chromatography with Ion Mobility Quadrupole Time of Flight Mass Spectrometry technology. Nineteen compounds were found to migrate to the soda from the nine samples analyzed with concentrations ranging values from 0.015 to 3.6 mg migrant/kg of soda. Variations in the compounds across obtained from three different manufacturers were found. These differences strongly suggest the use of different additives in the production of straws from the different manufacturers. Additionally, discrepancies in the compounds that migrated from the printed straws produced by one manufacturer were identified. Two photoinitiators, 2,2-dimethoxy-2-phenylacetophenone and diphenyl (2,4,6-trimethylbenzoyl)- phosphine oxide and a dye, rhodamine B were found to migrate from the soda to the straws. Particularly interesting was the migration of bis(2-ethylbutyl)phthalate and dioctyl phthalate, both recognized as endocrine disruptors, and 4,4'-methylenedianiline, a primary aromatic amine and suspected carcinogen, which had a migration concentration into the soda surpassing the specific migration limit set by Regulation (EU) No 10/2011. The study underscores that, despite straws not being made of plastic, several concerning compounds that migrated from them were additives commonly found in plastic products. This may suggest that paper straws may not be the safest alternative to plastic straws in terms of food safety.

1. Introduction

As a result of the implementation of Directive (EU) 2019/904 of the European Parliament and of the council of 5 June 2019 on the reduction of the impact of certain plastic products on the environment (European Union, 2019), a significant change has occurred in the area of single-use plastic straws. Plastic straws, which were once widely used, have been largely substituted with paper straws—a more environmentally conscious choice due to their biodegradability (Ahmed et al., 2018). There have been a number of studies examining the migration from paper to liquids (Rusko et al., 2020; Yuan et al., 2022); however the investigation of paper-based materials in this context has been comparatively limited and less extensive than with plastics (Martínez-Bueno et al., 2019; Nerin et al., 2018; Vera et al., 2018). The limited investigation is primarily due to the infrequent use of paper in direct contact with liquid food items, primarily due to its susceptibility to solubility. In particular, specific interactions between paper straws and various beverages, including soda, have yet to be thoroughly investigated. One particular aspect of interest is the ink content of many paper straws, that is used to create designs to enhance aesthetics and attraction for consumers. Inks have intricate formulations and comprise pigments or dyes, solvents, binders, and other additives all of which are meticulously blended to obtain the desired color, texture, adhesion, and print quality (Nerín et al., 2023; Pace, 2022). Amidst this complexity, certain components, particularly specific additives and unreacted monomers, could migrate from the inked surface into the surrounding environment.

The absence of harmonized regulation for paper, board, inks, and coatings as food contact materials within European regulations is

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notable. Resolution CM/Res (2020) 9, its Guiding Principles and the supplementary Technical Guides contribute to the protection of human health by ensuring, as defined in relevant European legislation, i.e. Regulation (EC) No. 1935/2004 (Commission Regulation (EU) No 1395/2004), the safety and quality of food contact materials and articles that are not covered by specific European legal provisions or other measures, e.g. at the European Union (EU) level (Council of Europe, 2020; Council of Europe, 2021; European Union, 2004). These mandates firmly dictate that FCMs must prevent the transfer of their constituents into food to an extent that could jeopardize human health or lead to undesirable alterations in food composition or sensory attributes. In simpler terms, the migration of potentially harmful substances from paper into food must be entirely prevented or kept within permissible limits.

However, certain European Union nations like Germany (Bfr XXXVI, 2023), France (MCDA, 2019), and the Netherlands (Bijlage deel, Hoofdstuk, 2023) possess distinct regulations related to paper and board in contact with food. Consequently, these regulations should also be considered as guiding principles.

Compliance with these regulations for printed straws necessitates the screening and subsequent identification of compounds migrating from the straws into the liquids with which they are used. However, achieving a comprehensive understanding of migration from printed straws presents a substantial challenge, primarily due to the identification of untargeted non-volatile compounds. The task involves the investigation and identification of previously untargeted substances that might migrate from the straws and relies on cutting-edge analytical methodologies, such as high-resolution mass spectrometry and advanced data analysis techniques (Martínez-Bueno et al., 2019; Nerin et al., 2013).

Ultra-High-Pressure Liquid Chromatography coupled to Ion Mobility Quadrupole Time of Flight Mass Spectrometry (UPLC-IM-Q/TOF) is a sophisticated analytical technique that combines the power of liquid chromatography with ion mobility separation and high-resolution mass spectrometry. This approach is particularly valuable for the identification of unknown compounds in complex samples. Ion mobility provides an extra orthogonal separation dimension, over more traditional mass spectrometry techniques, and ions can be separated by their drift times in addition to their mass-to-charge (m/z) values. This is particularly useful when studying complex samples such as beverages, since spectra with fewer interferences can be obtained by aligning precursor and fragment ions with respect to both their retention time in the chromatography column, and their drift time in the mobility cell. This method enables a higher degree of differentiation between analytes and potential matrix interferences, and has been successfully used to identify compounds in drinks matrices including tea, champagne, beer, wine or milk (Canellas et al., 2021, 2022; Hernández-Mesa et al., 2019; Karpas, 2013).

The use of statistical techniques to analyze the data obtained from ion mobility quadrupole time of flight mass spectrometry, enhances its analytical capabilities, making it a robust approach to explore intricate sample compositions and conduct comprehensive comparisons between them (Hou et al., 2023; Li et al., 2023; Lu et al., 2023; Lv et al., 2020).

The inherent capability of this technique to provide valuable information including retention times, accurate mass measurements, and collision cross-section (CCS) values presents the opportunity to establish comprehensive libraries of known compounds. Such libraries are an invaluable resource for identifying unfamiliar substances within specific domains such as food packaging. Therefore, the technique not only serves as a powerful tool for elucidating the identity of unknown analytes but also as a foundation for building a repository of spectral fingerprints that can be leveraged in the analysis of various samples across different contexts (Jariyasopit et al., 2022; Plachká et al., 2021; Song et al., 2022a).

Within the scope of this study, the innovative approach of integrating UPLC-IM-Q/TOF technology with advanced statistical analysis has been employed. The primary focus is the investigation of non-volatile migrants that are released from printed paper straws and subsequently migrate into soda. This comprehensive analytical method enables the identification and characterization of these migrants. Moreover, by assessing the potential risks inherent in the migration of these compounds, this research contributes valuable insights into the safety considerations of utilizing printed paper straws in conjunction with beverages.

Table 1
Samples studied, vendor, manufacturer name and number, country of manufacture and color of the straws.

Sample name	Vendor	Manufacturer name and number	Country of manufacture	Color
G 1	Opencor (Zaragoza, Spain)	Fackelmann (1)	China	Non printed
G 2	Opencor (Zaragoza, Spain)	Fackelmann (1)	China	Printed
G 3	Superbazar (Zaragoza, Spain)	Family menaje (1)	China	Non printed
G 4	Superbazar (Zaragoza, Spain)	Family menaje (1)	China	Black
G 5	Superbazar (Zaragoza, Spain)	Family menaje (1)	China	Pink
G 6	Makro (Zaragoza, Spain)	Makro profesional (3)	China	Non printed
G 7	Makro (Zaragoza, Spain)	Makro profesional (3)	China	Green striped
G 8	Makro (Zaragoza, Spain)	Makro profesional (3)	China	Red striped
G 9	Makro (Zaragoza, Spain)	Makro profesional (3)	China	Black striped

2. Materials and methods

2.1. Reagents and materials

Methanol of high-performance liquid chromatography (HPLC) grade was supplied by Scharlau Chemie S.A (Sentmenat, Spain). Deionized water was obtained from a MilliporeMilli-QPLUS 185 system (Madrid, Spain).

The reagents 2-[2-(benzoyloxy)ethoxy]ethyl benzoate (purity $>$ 95 %), tris(2,4-ditert-butylphenyl)phosphate (50 mg/L in acetonitrile), oleamide (purity $>$ 99 %), dioctyl phthalate (purity $>$99.5 %), bis(2-ethylhexyl) sebacate (purity $>$ 97 %), diisodecyl adipate (purity $>$ 99 %), 2-stearoylglycerol (purity $>$ 95 %), 2,2,4-trimethyl-1,3-pentanediol diisobutyrate (purity $\geq$ 98.5 %), 3-hydroxy-2,2,4-trimethylpentyl isobutyrate (purity 99 %), N,N-ethylenebis stearamide (purity $>$ 95 %), bis(2-ethylbutyl)phthalate (purity $>$ 99 %), 2,3-di(octanoyloxy)propyl octanoate (purity $\geq$97 %), 4,7,10,13,16,19-docosahexaenoic acid, methyl ester (purity $\geq$98 %), 2,2-dimethoxy-2-phenylacetophenone (purity 99 %), 3',6'-bis(diethylamino)spiro[isobenzofuran-1(3 H),9'-[9 H]xanthene]–3-one (purity $>$ 95 %), acetyl tributyl citrate (purity $\geq$ 98 %), diphenyl (2,4,6-trimethylbenzoyl)- phosphine oxide (purity $\geq$ 97 %), 4,4'-methylenedianiline (purity $\geq$ 97 %), 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-oxirane (purity $\geq$ 97 %) were purchased from Merck (Spain).

The soda utilized for migration studies was acquired from the Eroski supermarket. The product belonged to the Eroski brand and comprised of carbonated water, citric acid, sodium cyclamate, sodium saccharin, and various flavor components.

Straws were acquired from three local supermarkets: Opencor, Superbazar and Makro (Zaragoza, Spain). Details are shown in Table 1. The samples were individually covered with aluminum and stored at a temperature of 20 ºC until they were utilized for migration analysis.

2.2. Migration studies

Migration studies were done with a carbonated drink (soda). The migration studies were set-up according document by the European Commission's Joint Research Centre (Senaldi & Hoekstra, 2021). According to the document, the straws have to be placed into contact with the food for 0.5 h at 70 ºC. Moreover, the ratio surface to amount of food established by the document is 6 dm^2 to 1 kg of food, with total immersion. Then, 0.12 dm^2 were place into contact with 0.02 kg of soda. Three replicates of each sample were prepared and analyzed. Moreover, three replicates of the blanks consisting of degasified soda were prepared and analyzed.

2.3. Ultra-high-pressure-liquid chromatography coupled to ion mobility-quadrupole time of flight analyzer (UPLC-IM-Q/TOF)

The study utilized a Waters Acquity™ UPLC chromatography system coupled to an electrospray interface (ESI) and Vion® ion mobility-quadrupole time of flight (IMS/Q/TOF) mass spectrometer located in Manchester, UK for screening analyses. The UPLC BEH C18 column measuring 2.1 × 100 mm with 1.7 μm particle size was employed with a flow rate of 0.3 mL/min and a column temperature of 35 ºC.

The non-targeted study was done with water (phase A) and methanol (phase B), both containing 0.1 % formic acid. The gradient started at 95 % A and increased to 100 % B over 13 min, followed by 2 min of re-equilibration to initial conditions. A volume of 5 μL of sample was injected.

The ESI source was utilized in positive and negative ionization mode with a capillary voltage of 3 kV and a sampling cone of 30 V in sensitivity mode. The source block and desolvation gas were set to temperatures of 120 °C and 500 °C, respectively, and the desolvation gas flow rate was 800 L/h. The mass range of acquisition was 50–1000 *m/z*, and Leucine-Enkephalin [M+H]+, *m/z* 556.2766 [M+H]-, 554.2615 *m/z*, was utilized as the lock-mass compound for real-time mass correction. The study utilized high definition MS^E mode ($HDMS^E$) in data independent analysis (DIA) with low collision energy (6 V) and high collision energy (ramp from 20 V to 40 V) data collected simultaneously. Argon served as the collision gas and nitrogen was the ion-mobility gas. The IMS gas flow rate was 25 mL/min, wave velocity 250 m/s, and IMS pulse height 45 V. Calibration of both mass and CCS was conducted utilizing Major Mix kit from Waters Corp. The acquisition rate was 10 Hz, and UNIFI v.1.8 software was used for data acquisition and processing. The analysis method utilized for target identification was based on the Song et al. database (Song et al., 2022a, 2022b) and involved a retention time tolerance of 0.2 min, mass target tolerance of 5 ppm, and collision cross tolerance of 5 %.

Migration samples were directly analyzed. Pure standards were used to spike degasified soda to obtain recoveries, limits of detection and external calibration curves. 1000 μg/g of each standard was initially prepared in degasified soda and dilutions of the solutions in degasified soda were prepared. Lineal range used for calibration, limits of detection and limits of quantification are shown in Table 2. The limit of detection (LOD) and limit of quantification (LOQ) of the analytes were calculated by the calibration curve procedure using the slope and standard deviation of regression.

3. Results and discussion

3.1. UPLC-IM-Q/TOF

The migration solutions obtained, were analysed using UPLC-IM-Q/TOF since this technique offers an extra degree of separation, over more traditional mass spectrometry analyses, in the form of drift time. In the subsequent analysis of the data, interferences from coeluting compounds and complex matrices, can be dramatically reduced by aligning precursor and fragment ions in both the retention time and drift time dimensions.

Three replicates of each sample were analyzed and the data form each were processed by performing peak detection followed by componentization, which utilized both retention time and drift time alignment. The resulting components were collated across the complete sample set and subjected to Principal Component Analysis (PCA) simply to determine whether there were any differences between the sample groups. The statistical software package EZInfo (Sartorius), which is integrated with UNIFI and affords seamless, two-way data transfer, was used for the statistical treatment of the data. Criteria for the selection of the most significant markers (outliers on the scores plot) were p[1] (loadings) $> |0.07|$ and p(corr)[1] (correlation) $> |0.97|$. TIC normalization and Pareto scaling were chosen for data preprocessing prior to PCA/OPLS-DA.

The scores plot from the PCA (Fig. 1) shows that samples G1 and G2 group together, as do samples G3 and G5, and samples G6 to G9 and each of these groups contain samples from a single manufacturer (see Table 1). The G4 samples, supplied by the same manufacturer as samples G3 and G5, are clearly in grouped alone which demonstrates the compounds migrating from these samples are different to those from other straws from the same supplier.

In order to determine the compounds, or markers, responsible for the differences between the G3 and G4 sample groups, an Orthogonal Projection to Latent Structures Discriminant Analysis (OPLS-DA) was performed and the resulting S-Plot is shown in Fig. 2. The S-plot combines the covariance of the markers (x-axis) and correlation of the markers (y-axis) from the OPLS-DA on a scatter plot. Markers that are only present in one of the sample groups, or elevated in a sample group, occupy the regions $y = 1$ and $y = -1$ on the S-plot. Fig. 2 highlights three markers observed exclusively, or at elevated levels, in sample G4. These markers represent compounds that exhibited unique migration patterns from sample G4 and were put forward as candidates for identification. Identification of the compounds within the samples was achieved using two distinct methodologies. Firstly, the test samples underwent a screening process utilizing the comprehensive database of food contact material compounds developed by Song et al. (Song, Canellas, Dreolin, Goshawk, & Nerin, 2022a,b; Song, Dreolin, Canellas, Goshawk, & Nerin, 2022c). Currently, this extensive database encompasses a substantial collection of 10,181 compounds, including both frequently employed additives and non-intentionally added substances that are commonly encountered within food contact materials. The database is dynamic and continues to expand over time. It is noteworthy that this compilation includes valuable data not solely limited to Collision Cross Section (CCS) values, but also incorporates pertinent metrics like retention time and precise mass measurements.

The capability of the UNIFI software employed in this study, lies in the automated capacity to correlate and assign compounds migrating from the straws into the soda. This software effectively cross-references the retention time, accurate mass, and CCS values of the measured data against the wealth of information contained within the database, ensuring conformity with the tolerances specified in Section 2.3. To validate the confirmatory aspect of the analysis, data for authentic pure standards were obtained.

Table 2 lists the identified compounds within the migration solutions. It includes details such as the sample ID, limit of detection (mg/kg), CAS number, specific migration limit, and calculated specific migration limit as per the Cramer classes. Moreover, the table provides information on retention time and the variance in retention time compared to the database retention time (in minutes) for compounds recognized via the database library approach. For compounds identified using the same methodology, the table lists the detected *m/z* values and

Table 2

Name of the compounds identified by UPLC-IM/QTOF, sample number, limit of detection (LOD), CAS number, specific migration limit according Regulation (EU) No 10/2011or proposed specific migration limit (SML) according TTC concept, retention time and difference between database retention time and experimental retention time (min), *m/z* detected experimentally difference between database *m/z* and experimental *m/z* (mDa), CCS obtained experimentally and difference between database CCS and experimental CCS expressed (delta CCS%) and identification through library or through fragmentation.

Compound name	Sample	LOD mg/kg	LOQ mg/kg	Lineal range mg/kg	CAS	SML Regulation (EU) No 10/2011	Proposed SML TTC mg/Kg	Retention time (min) Δrt (min)	*m/z* detected (Da) $\Delta m/z$ (mDa)	CCS (Å^2) ($\Delta CCS\%$)	Adduct	Main fragments
2-[2-(benzoyloxy)ethoxy] ethyl benzoate	G4	0.05	0.17	0.17-1.5	120-55-8		1.8	8.23	315.1230	172.76*	H^+ Na^+	149.0603, 105.0342
tris(2,4-ditert-butylphenyl)phosphate	G3,G4,G5	0.01	0.03	0.03-0.5	95906-11-9		0.09	9.5 (0.18)	685.4361 (0.2)	283.29 (0.76)	Na^+	
oleamide	G1,G2	0.01	0.03	0.03-1.0	301-02-0	60		10.1	282.2792	185.61	H^+	265.2528, 247.2430, 123,1172, 97.1021
dioctyl phthalate	G4	0.02	0.07	0.07-1.5	117-84-0		1.8	10.4	390.2727	218.54	H^+	167.0342, 149.0236, 71.0866
bis(2-ethylhexyl) sebacate	G3,G4,G5	0.03	0.10	0.10-1.5	122-62-3		1.8	8.6 (0.0)	449.3611 (1.3)	229.58 (1.75)	Na^+	
diisodecyl adipate	G6, G7, G8,G9	0.02	0.07	0.07-1.5	27178-16-1		1.8	8.6 (0.12)	449.3616 (2.1)	232.29 (0.89)	Na^+	
2-stearoylglycerol	G6, G7, G8,G9	0.06	0.20	0.20-3.0	621-61-4		1.8	8.05 (0.10)	381.2966 (0.9)	202.66 (2.10)	Na^+	
2,2,4-trimethyl-1,3-pentanediol diisobutyrate	G1,G2	0.05	0.17	0.17-5.0	6846-50-0	5		7.10 (0.13)	309.2333 (0.1)	177.65 (0.98)	Na^+	
3-hydroxy-2,2,4-trimethylpentyl isobutyrate	G1,G2	0.06	0.20	0.20-1.5	25265-77-4		0.54	8.31	217.1801 (2.6)	157.00*	H^+ Na^+	199.1693, 129.1276, 111.1172, 89.0606
N,N-ethylenebis stearamide	G1,G2	0.03	0.10	0.10-3.0	110-30-5	60		9.5 (0.09)	615.5797 (2.4)	279.00 (0.79)	Na^+	
bis(2-ethylbutyl)phthalate	G3,G4,G5	0.05	0.17	0.17-1.5	7299-89-0		1.8	7.75 (0.09)	357.2038 (2.1)	196.47 (1.23)	Na^+	
2,3-di(octanoyloxy)propyl octanoate	G6,G7, G8,G9	0.04	0.13	0.13-2.0	538-23-8		1.8	8.4 (0.11)	493.3520 (0.8)	230.6 (0.97)	Na^+	
4,7,10, 13,16,19-docosahexaenoic acid, methyl ester	G3,G4,G5	0.03	0.10	0.10-1.0	301-01-9		1.8	8.1 (0.05)	365.2451 (1.8)	192.5 (1.36)	Na^+	
2,2-dimethoxy-2-phenylacetophenone	G3,G4,G5	0.03	0.10	0.10-1.0	24650-42-8		0.09	5.82 (0.14)	279.0992 (0.7)	157.6 (0.23)	Na^+	
3',6'-bis(diethylamino)spiro[isobenzofuran-1 (3H),9'-[9H] xanthene]-3-one	G4	0.01	0.03	0.03-0.5	509-34-2		0.09	4.58	465.2149 (0.3)	219.3	Na^+	
acetyl tributyl citrate	G6,G7, G8,G9	0.01	0.03	0.03-2.0	77-90-7	60		6.93	425.2146 (1.0)	204.02	Na^+	
diphenyl (2,4,6-trimethylbenzoyl)- phosphine Oxide	G6,G7, G8,G9	0.01	0.03	0.03-1.0	75980-60-8		0.09		371.1171 (0.1)	186.87	Na^+	
4,4'-methylenedianiline	G3,G4,G5	0.003	0.01	0.01-0.3	101-77-9 -	0.01		1.53	199.1230 (0.4)	158.25	H^+	106.0656
2,2'-[(1-methylethylidene)*bis*(4,1-phenyleneoxymethylene)] *bis*-oxirane	G3,G4,G5	0.02	0.06	0.06-3.0	1675-54-3	1		6.4	363.1567 (0.2)	174.26	Na^+	

* CCS value from H^+ adduct

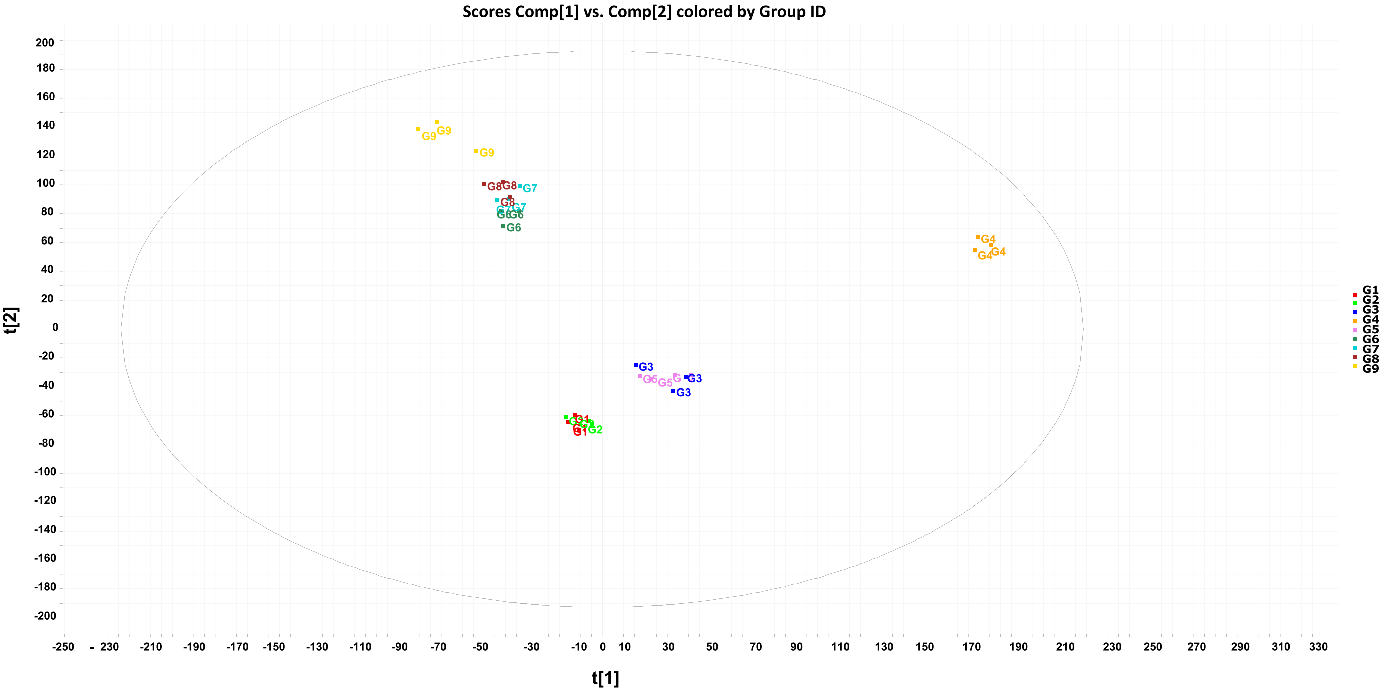

Fig. 1. Scores plot obtained from the Principal Component Analysis for the three replicates of each sample analyzed.

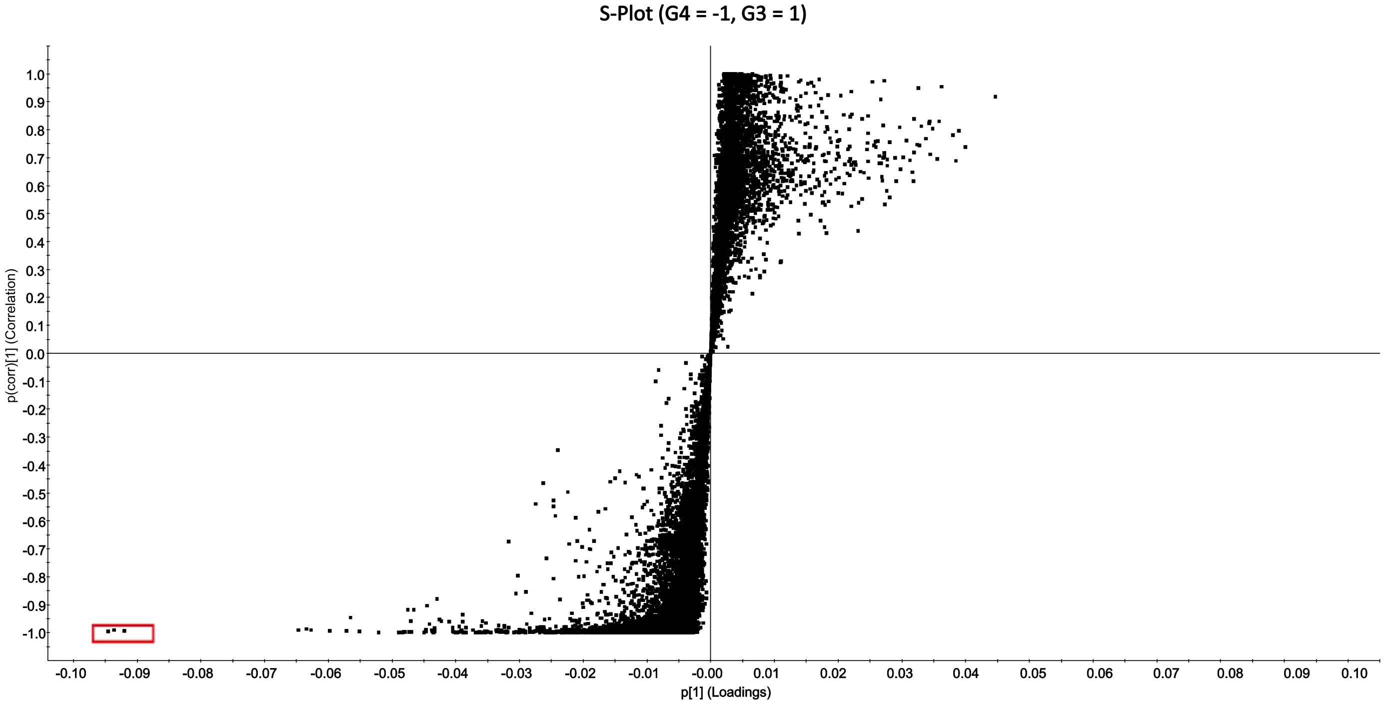

Fig. 2. Orthogonal Projection to Latent Structures Discriminant Analysis (OPLS-DA) S-plot obtained to compare the sample G4 (left side) against the sample G3 (right side).

the variance in *m/z* between the database and experimental values. Additionally, CCS values along with the percentage difference between database CCS and experimental CCS (CCS delta %) are presented. The table also presents the detected adducts and primary fragments for each compound.

The outcomes of this procedure, as evidenced in Table 2, unveiled the successful identification of the compounds tris(2,4-ditert-butylphenyl)phosphate, bis(2-ethylhexyl) sebacate, diisodecyl adipate, 2-stearoylglycerol, 2,2,4-trimethyl-1,3-pentanediol diisobutyrate, N,N-ethylenebis stearamide, bis(2-ethylbutyl)phthalate, 2,3-di(octanoyloxy)propyl octanoate, 13,16,19-docosahexaenoic acid, methyl ester, 2,2-dimethoxy-2-phenylacetophenone, 3’,6’-bis(diethylamino)spiro[isobenzofuran-1(3 H),9’-[9 H]xanthene]–3-one, acetyl tributyl citrate, diphenyl (2,4,6-trimethylbenzoyl)- phosphine oxide, 4,4’-methylenedianiline and 2,2’-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-oxirane. It is intriguing to note that the identification of all these compounds was facilitated through their association with the sodium adduct with the exception of 4,4’-methylenedianiline. Due to their limited propensity for fragmentation, sodium adducts do not exhibit fragment ions, as evidenced by the absence of fragments in Table 2. This characteristic poses a significant challenge in terms of identifying compounds solely through fragmentation patterns. Consequently, the significance of the libraries employed in this study, which rely on retention time, precise mass, and CCS, is underscored by this very aspect.

In cases where identification through the prescribed procedure was not possible, an alternative approach was used using experimentally derived fragmentation patterns. This complicated process involved several steps, starting with the molecular ion extracted from the low-energy spectrum. This molecular ion served as the foundational element to propose an elemental composition, using an i-fit confidence threshold of no less than 80 %. To derive the elemental composition, a comprehensive range of elements including carbon, oxygen, hydrogen, nitrogen, chlorine, bromine, sulfur, and phosphorous were judiciously considered.

To proceed with the identification, we utilized the ChemSpider database, which assisted in locating molecules that matched the elemental composition. Delving deeper, the Fragment Match tool (tool included in the UNIFI v.1.8 software) emerged as a key player in this process. This tool adeptly orchestrated a comparison between the meticulously gathered accurate mass measurements and the theoretical fragments characteristic of each proposed molecular candidate.

To confirm the identification, pure standards were analyzed. This method combines experimental patterns, advanced database searches, and theoretical fragment comparisons, showcasing its complex yet thorough nature. Fig. 3 illustrates the identification of the compound 3-Hydroxy-2,2,4-trimethylpentyl isobutyrate using this procedure. The figure displays both the low and high energy spectra. In the low energy spectrum, the hydrogen adducts corresponding to the *m/z* 217.1801 and the sodiated adduct corresponding to the *m/z* 239.1617 were observed. Moreover, fragmentation was obtained in the low energy spectrum obtained with the conditions described in the 2.3. section. The fragments observed matched with a fragment of the theoretical candidate proposed. In the high energy spectrum, the hydrogen adducts almost disappeared due to its high tendency to be fragmented. More fragments were observed in the high energy spectrum as the collision ramp was applied. It can be seen that the highest fragments observed in the low energy spectra such as *m/z* 199.1593 and 129.1276 have been fragmented resulting in lower *m/z* fragments. Nevertheless, since sodiated adducts have lower tendency to fragment, the sodiated adduct could be observed in the high energy spectrum. All the fragments obtained experimentally matched with the fragments of the candidate proposed. Four compounds were identified following this procedure, 3-hydroxy-2,2,4-trimethylpentyl isobutyrate, oleamide, dioctyl phthalate and 2-[2-(benzoyloxy)ethoxy]ethyl benzoate.

The screening analysis employed in this study aimed to visualize a wide range of analytes migrating from printed paper straws into soda. However, there are several constraints in the methodology that warrant

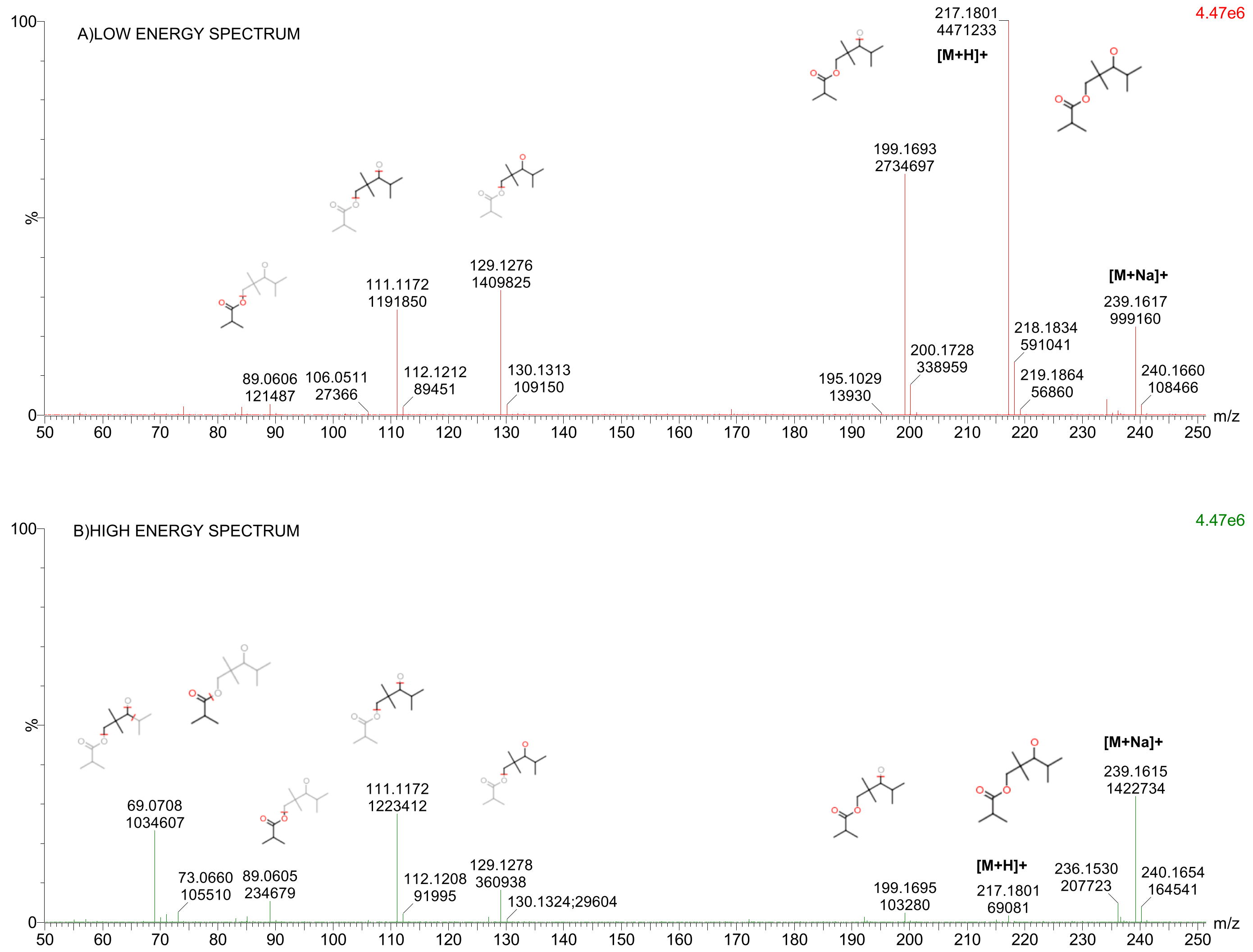

Fig. 3. Low energy spectrum (A) and high energy spectrum (B) obtained for the compound 3-Hydroxy-2,2,4-trimethylpentyl isobutyrate.

consideration. Limitations in negative ESI mode, particularly when using eluents with formic acid, may result in insufficient ionization of certain compound classes, such as bisphenols, making them undetectable. Additionally, compounds like chloro propanols found in wet strength paper FCMs may not be identified through LC-MS analysis. The study focused on a single aqueous matrix with a slightly acidic pH, limiting the generalizability of migration dynamics. The exploration of alternative matrices, such as alcoholic beverages with diverse pH levels, could provide additional insights. While a comprehensive exploration was aimed for in our approach, the boundaries of our methodology are emphasized by these limitations, and understanding could be enhanced in future studies by addressing these constraints.

Upon the conclusion of the identification process, the subsequent step involved quantification. This entailed creating calibration curves through the injection of standard compounds that had been identified earlier. Detailed information regarding the limits of detection can be found in Table 2, along with the specific migration limits that have been established in accordance with Regulation (EU) No 10/2011 and the proposed specific migration limits calculated according Threshold of Toxicological Concern (TTC) concept (EFSA, 2019). These limits serve as provisional values for ensuring the safety and compliance of the analyzed substances.

The utilization of specific migration limits established by Regulation (EU) No 10/2011 stems from the absence of harmonization for paper and board within European legislation regarding food contact materials. Given this regulatory gap, Regulation (EU) No 10/2011 plays a pivotal role in guiding the assessment of materials intended for contact with food. By establishing precise limits for the migration of substances from plastic food contact materials, into food, the regulation provides a standardized framework for ensuring the safety of consumers. In the case of paper and board, which lack harmonized regulations, the application of these specific migration limits serves as a valuable reference point to ascertain the permissible levels of migration, thereby safeguarding the health and well-being of individuals who consume food that comes into contact with these materials. Nevertheless, some of these compounds, as shown in Table 2, are not listed in Regulation (EU) No 10/2011 (Commission Regulation (EU) No 10/2011, 2011). In spite of that, according the Regulation (EC) No 1935/2004 (Commission European Union. (2004), manufacturers must evaluate any potential health risks in the final product, using internationally recognized scientific principles on risk assessment. This evaluation, following the guidance proposed by European Food Safety Authority can involve applying the TTC concept (EFSA, 2019). The classification is a risk assessment tool used to evaluate the safety of chemical substances based on their two-dimensional structure and potential exposure levels, just in case of lacking toxicity data. The TTC concept categorizes compounds into different classes and assigns them specific exposure limits. These exposure limits are based on the principle that substances can be safely consumed at very low levels, provided they fall below a certain threshold of toxicity. The TTC sets exposure limits, as described by Kroes et al. (2004).

Table 2 shows the migrants coming from the different samples which were obtained from various manufacturers as indicated in Table 1. Fig. 4, shows the migration values expressed as mg/kg and the specific migration limits obtained by regulation and Cramer classes (Commission Regulation (EU) No 10/2011, 2011; Kroes et al., 2004).

Concerning samples G1 and G2, migration of the compounds oleamide, 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate, 3-hydroxy-2,2,4-trimethylpentyl isobutyrate and N,N-ethylenebis stearamide was observed. hese compounds are used in coatings and plastics (Groh et al.,

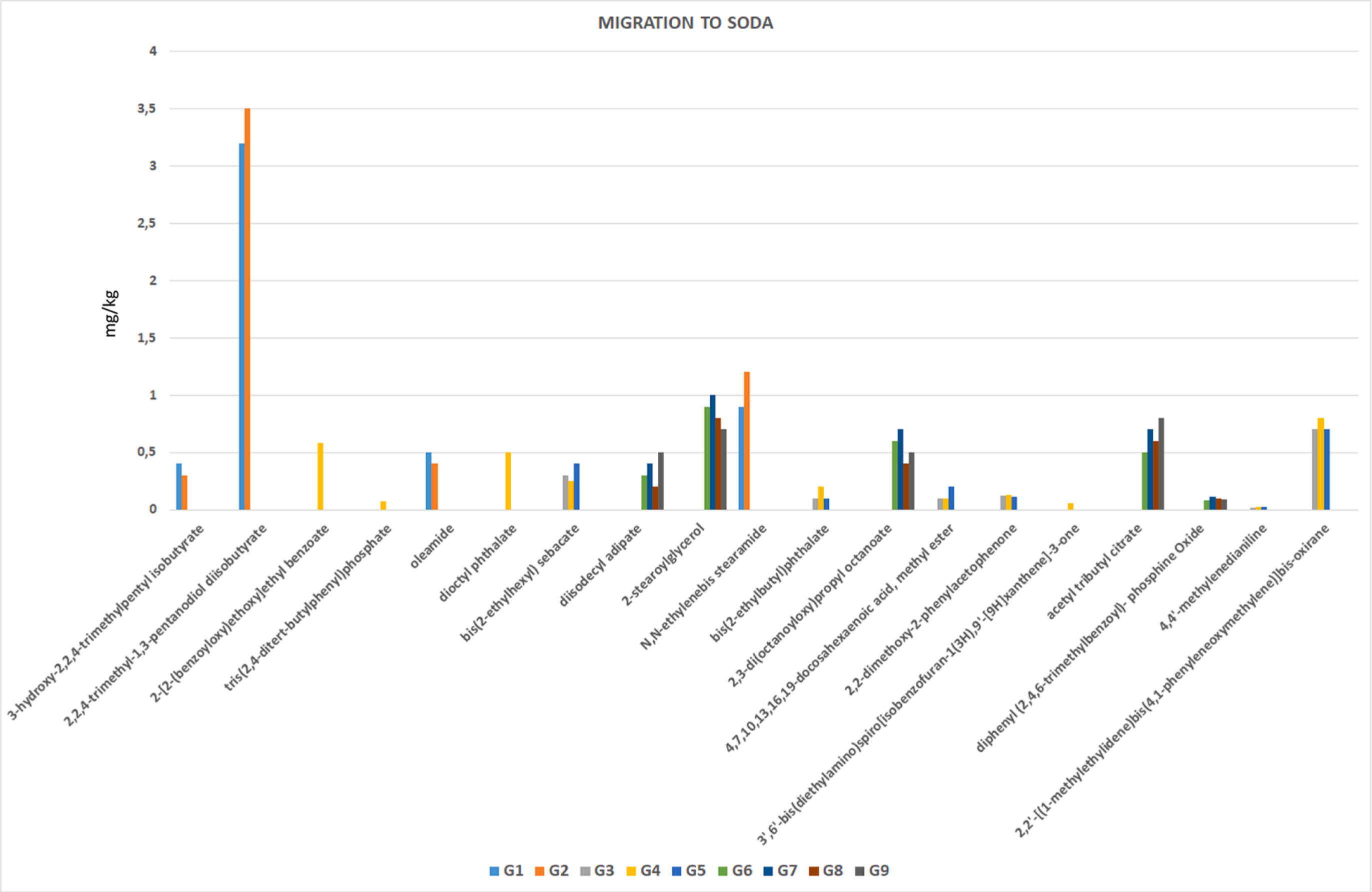

Fig. 4. Migration values of the identified compounds migrating from straws to soda expressed in mg/kg.

2021a). The compounds oleamide, 3-hydroxy-2,2,4-trimethylpentyl isobutyrate, and N,N-ethylenebis stearamide have never been observed migrating from paper packaging (FCCmigex Database, 2023). However, the compound 2,2,4-trimethyl-1,3-pentanediol diisobutyrate has been observed to migrate from polyethylene-coated paper (Pack et al., 2021).

The migration of the compounds from straws G1 and G2 to soda was below the limits (Fig. 4, Table 2). The SML of the compounds oleamide, N,N-ethylenebis stearamide and 2,4-trimethyl-1,3-pentanediol diisobutyrate was 60 mg/kg, 60 mg/kg and 5 mg/kg respectively according Regulation (EU) No 10/2011 (mg/Kg). According Fig. 4 and Table 2, their migration was below its limit. Moreover, the proposed specific migration limit calculated from the TTC concept was 0.54 mg/kg. As can be seen in Fig. 4, the migration was below this limit.

Bis(2-ethylhexyl) sebacate, bis(2-ethylbutyl)phthalate, 2,2-dimethoxy-2-phenylacetophenone, 4,4’-methylenedianiline, 2,2’-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-oxirane and 4,7,10,13,16,19-docosahexaenoic acid methyl ester, tris(2,4-ditert-butylphenyl)phosphate, were found to migrate from all the samples obtained from the manufacturer 2 (G3, G4 and G5).

Bis(2-ethylhexyl) sebacate, and 4,7,10,13,16,19-docosahexaenoic acid, methyl ester are common additives used in coatings and inks (Groh et al., 2021a). Tris(2,4-di-tert-butylphenyl) phosphate is a non-intentionally added substance (NIAS) produced by the oxidation of the compound Irgafos 168, a common antioxidant (Vera et al., 2018). These compounds typically do not migrate from paper; however, they commonly migrate from plastics and coatings ((FCCmigex Database, 2023). The substances were categorized as Cramer class I, and their migration remained below the proposed Specific Migration Limit (SML) according to the Threshold of Toxicological Concern (TTC) concept, which was set at 1.8 mg/kg (see Fig. 4).

The compound 2,2’-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bis-oxirane commonly known as BAGDE is additive or starting agent used in plastics, coatings, sealing and adhesives (European Chemical Agency, 2023a). This compound has been previously identified as migrating from recycled paper (Perez-Palacios et al., 2012). The compound migrated below their SML (1 mg/kg) according Regulation (EU) No 10/2011 (Fig. 4).

Concerning the compound 2,2-dimethoxy-2-phenylacetophenone is a photoinitiator used in printing inks (Groh et al., 2021a). The compound was recently documented to migrate from food paper packaging materials (Liang et al., 2022). The substance was assigned to Cramer class III, and its migration stayed beneath the proposed Specific Migration Limit (SML) as per the Threshold of Toxicological Concern (TTC) concept, set at 1.8 mg/kg (Fig. 4).

Regarding the compound bis(2-ethylbutyl)phthalate, despite its migration being below its proposed migration limit according TTC concept (1.8 mg/kg), is included in a list of 608 hazardous substances that have been prioritized as the most urgent candidates for further evaluation according Groh et al. (Groh et al., 2021b) that explored FCCdb chemicals’ hazards using several authoritative sources of hazard. The compound is considered as an endocrine disruptor (Latini et al., 2004). This substance generally does not exhibit migration from paper; nevertheless, it frequently migrates from plastics and coatings (FCCmigex Database, 2023).

A very important consideration must be made regarding the migration of the compound 4,4’-methylenedianiline. The present compound is a primary aromatic amine recognized as carcinogenic (European Chemical Agency, 2023b), and it has exceeded the allowable limit (Commission Regulation (EU) No 10/2011, 2011) in all samples from G3 to G5. Like the previously identified compound, it is more frequently detected as migrating from plastics, adhesives, or inks.

Moreover, as it could be seen in the Fig. 1, sample G4 (black straw) was statistically different from samples G3 (white straw) and G5 (pink straw) from the same manufacturer. The substances 2-[2-(benzoyloxy)ethoxy]ethyl benzoate, 3’,6’-bis(diethylamino)spiro[isobenzofuran-1(3 H),9’-[9 H]xanthene]–3-one, and dioctyl phthalate exclusively migrated from sample G4. 2-[2-(Benzoyloxy)ethoxy]ethyl benzoate is a plasticizer in plastics, inks and coatings (European Chemical Agency, 2023c). It has been previously identified as migrating from food packaging made of paper (Sapozhnikova, 2021). 3’,6’-bis(diethylamino)spiro[isobenzofuran-1(3 H),9’-[9 H]xanthene]–3-one is a dye, previously identified as migrating from paper to food contact materials (Bengtström et al.,2016). Finally, dioctyl phthalate, a plasticizer, has been shown to migrate from plastics (Bonini et al., 2008), coatings, and inks but not from paper samples (Carlos et al., 2021). Therefore, it can be inferred that the coating or polymer used for printing in sample G4 may be different from that used in samples G3 and G5.

These compounds werent́ listed on Regulation (EU) No 10/2011 (Commission Regulation (EU) No 10/2011, 2011). Therefore, TTC concept was applied as explained before. As can be observed in Fig. 4, migration of the compounds 2-[2-(benzoyloxy)ethoxy]ethyl benzoate and 3’,6’-bis(diethylamino)spiro[isobenzofuran-1(3 H),9’-[9 H]xanthene]–3-one was below the proposed specific migration limit(Cramer class I, SML 1.8 mg/kg). Nevertheless, the compound dioctyl phthalate, despite its migration being below its proposed migration limit according TTC concept (1.8 mg/Kg) is included in the list of 608 hazardous substances that have been prioritized as the most urgent candidates for further assessment and substitution in food contact materials as is an endocrine disruptor (Qureshi et al., 2016). This underscores the significance of monitoring the migration of this compound.

The compounds diisodecyl adipate, 2-stearoylglycerol, acetyl tributyl citrate, and 2,3-di(octanoyloxy)propyl octanoate that are additives used in coatings, adhesives and plastics migrated from all the samples obtained from manufacturer 3 (G6–9). Except for acetyl tributyl citrate (Wang et al., 2015), none of these compounds have ever been observed migrating from paper (FCCmigex Database, 2023).

Furthermore, the photoinitiator diphenyl (2,4,6-trimethylbenzoyl)-phosphine oxide also migrated from these samples. This compound has been documented to migrate from food packaging materials with a paper base (Liu, 2019). All these compounds migrating from samples G6–9 to soda weren`t present in the Regulation (EU) No 10/2011 (Commission Regulation (EU) No 10/2011, 2011). They were classified in the Cramer class I with a proposed specific migration limit of 1.8 mg/kg according the TTC concept. The migration observed was below their proposed specific migration limits.

It is imperative to direct a heightened level of attention towards the compounds, 4,4’-methylenedianiline, bis(2-ethylbutyl)phthalate and dioctyl phthalate found in samples contaminated by straws from manufacturer 2, due to their significant implications. These phthalates have been identified as part of a list encompassing 608 hazardous substances, making their migration from samples originating from manufacturer 2 a matter of considerable concern. These flagged substances warrant deeper investigation to comprehensively assess their potential impact on consumer safety.

4. Conclusions

The combination of the advanced analytical technique UPLC-IM-Q/TOF with Principal Component Analysis (PCA) and Orthogonal Projection to Latent Structures Discriminant Analysis (OPLS-DA) allowed a comprehensive analysis of the data, with Accurate Mass/Retention Time pairs playing a vital role in discerning patterns within the dataset. Notably, PCA demonstrated its effectiveness in distinguishing between suppliers, and even within the same supplier based on ink composition. The divergence of sample G4 from the other samples obtained from the same manufacturer further emphasized the influence of ink on migration dynamics. Moreover, The S-plot within OPLS-DA effectively identified markers driving significant discrepancies.

In conclusion, this holistic approach revealed specific compounds of concern and emphasized potential safety issues related to certain migrating substances. The study highlights that, a number of concerned compounds that migrated from the paper straws were additives typically found in plastic products. This raises the possibility that paper straws may not offer a safer alternative to plastic straws in terms of food safety. Then it has prompted the necessity for further research and careful deliberation regarding the adoption of paper straws.

CRediT authorship contribution statement

Goshawk Jeff: Resources, Software, Writing – original draft, Writing – review & editing. **Nerin Cristina:** Funding acquisition, Resources. **Dreolin Nicola:** Resources, Software, Writing – original draft, Writing – review & editing. **Vera Paula:** Conceptualization, Investigation, Methodology, Supervision, Writing – original draft, Writing – review & editing. **canellas elena:** Conceptualization, Investigation, Methodology, Resources, Supervision, Writing – original draft, Writing – review & editing, Funding acquisition, Project administration.

Declaration of Competing Interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Elena Canellas reports a relationship with the grant RYC2021-034150-I funded by MCIN/AEI/ 10.13039/501100011033 and by the "European Union Next Generation EU/PRTR that includes: funding grants and paid expert testimony.

Data Availability

Data will be made available on request.

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