A NON-TARGETED APPROACH TO THE DEVELOPMENT OF A FOOD ADDITIVE CCS SCREENING LIBRARY AND ITS APPLICATION

OVERVIEW

A targeted UPLC-MS for mobility sensitivity to generate HDMS (precursor ion, product ion) CCS library has been used to create a food additive MS library that has been performed.

- The food additives library generated incorporates, sweeteners, food colourings, antioxidants, and preservatives.

- Extracts of food and drinks products labelled as containing food additives have been analysed in triplicate using the HDMS CCS library generated.

- Compared to the food additive CCS library, the data values of < 2% have been considered satisfactory using both positive and negative ion modes.

INTRODUCTION

Although the use of food additives is strictly regulated under various EU directives, numerous studies have shown a potential for false positive and negative identifications. In order to enhance detection and confirm the monitoring of food additives, ion mobility mass spectrometry (IM-MS) is being increasingly utilized. Immunological methods are compulsory and are done to be identified and classified as to positive/negative additives. This method is considered a powerful method for the detection of food additives. It is non-invasive, particularly when used to perform a rapid analysis of food samples. In addition, it is easy to control and can also be used to detect exposure time, to threshold levels to be controlled. Hence, the development of a IM-MS is a great need.

According to the EU legislation, any new “substance” or substances that can somehow contain or use food in itself and not necessarily used as a chromatographic technique, is considered a food additive, and the introduction of the same are approved by the European Commission after being authorized by the European Commission. This approach is not considered to be an easy task. The challenges are mainly in the development of a high-throughput, high-throughput method, which is able to handle large numbers of samples, allowing for large-scale studies. This is of crucial importance to ensure that the food products are safe for consumption within the country. The factors for which are food contains certain additives or the absence of it. The goal is a method that can be used to identify food in its entirety. Water-based systems are used to identify food in its entirety. The system is designed to be essentially a development of aion mobility mass spectrometry (IM-MS) of food additives.

METHODS

- UPLC-MS: Waters System: Spectra-Smart 50 H. Electrospray positive (ESI) and negative (ESI-). Desolvation temperature (50°C). Desolvation air (50 L/min). Capillary voltage (3 kV). Waters Acquity UPLC (50 mm x 2.1 mm, 1.7 µm).


RESULTS AND DISCUSSION

A collision cross-section for food additives has been developed using the non-targeted mobility mass spectrometry technique. This method can be used to identify both the food additives and the food products. Further, ion mobility mass spectrometry is used to generate confident product ions and confirm the mobility values of the food additives. The food additives can be identified using food additives libraries.

- FOOD COMMODITY ANALYSIS UPLC METHOD

For the analysis of milk, the mobile phase was 18.0 mL min acetate 0.1% Formic Acid (A) and 18.0 mL min acetonitrile 0.1% Formic Acid (B) and mobile phase was gradient 1 min (98:2 A:B) 5.5 min (92:8 A:B) 7 min (92:8 A:B) 9 min (100:0 A:B). The sample was acquired in positive and negative ion modes on an acuity ultra performance liquid chromatography (UPLC) system and the water-based system was performed using the Waters MS Vision software.

- LIBRARY GENERATION UPLC METHOD

- Mobile phase: A water 18.0 mL min acetate 0.1% Formic Acid (A) and 18.0 mL min acetonitrile 0.1% Formic Acid (B) and mobile phase was gradient 1 min (98:2 A:B) 5.5 min (92:8 A:B) 7 min (92:8 A:B) 9 min (100:0 A:B). The sample was acquired in positive and negative ion modes on an acuity ultra performance liquid chromatography (UPLC) system and the water-based system was performed using the Waters MS Vision software.

- Extraction: and Sample Preparation

Food commodities covered for food additives: red fruits yoghurt (YB); sweetened white yogurt (YB); red fruits yoghurt (YB); red fruits yoghurt (YB), and lemonade drink (D5). The samples were prepared using the following extraction method. A 5-g mass of each commodity was introduced into a centrifuge tube (50 mL) containing MgSO₄ (6 g) and sodium acetate (1.52 g) were added to the tube, to induce phase separation. Samples were immediately shaken for 1 min, and then centrifuged for 5 min at 1500 rcf at 4°C. After centrifugation, 10 mL of the supernatant solution was collected using syringe for LC/MS analysis (Nano-HPLC) and QqQ-MS system. The solution was injected into an LC system for separation and the mobile phase was gradient.

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