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Mass Spectra 2018: HS-GCMS-SIM mode method template for identification of varieties of anionic, cationic and neutral surfactants as SIM-fingerprint-ID- Chong Mun Hwa - Synthomer Plc

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Surfactants play an important role in reducing surface tension, as it enables the control interfacial tension between liquids or solid-liquids. The application has been increasing worldwide and safety concern regarding the long term exposure to surfactant has been long discussed. Hence, the identification of surfactants in final products is crucial. The new method has been developing in Head-Space Gas Chromatography Selected Ion Monitoring mode (HS-GCMS-SIM mode) allowed the collection of surfactants as SIM-fingerprint-ID. The advantage of the method is it applies to broad range surfactants containing different chemistries. In addition, the analyses incorporate green chromatographic technique which reduces environmental impact/pollution with simple sample preparations. This database allows direct identification of the types of surfactants without derivatization, fast analysis time and ability of low concentration tracing. A novel headspace gas chromatography-mass spectrometry (HS GC-MS) method was developed for analysis of volatile compounds in onion (Allium cepa L. var. cepa, 'Recas'). MS was operated using full scan mode and selective ion monitoring (SIM) mode in order to quantify some specific compounds with increased sensitivity relative to full scan mode. The limits of detection and quantitation ranged from 0.01 to 0.10 µg/g and from 0.02 to 3.83 µg/g fresh weight, respectively, for studied compounds. The procedure allowed the identification of eighteen compounds and quantitation of nine compounds in the volatile fraction of onion, belonging mainly to di-, and trisulfides and aldehydes. These methods were applied to evaluate how high-pressure (HP) as a processing technology affects onion volatile compounds, responsible in part of the onion biological activity. Onion samples were treated at T1: 200 MPa/25°C/5 min, T2: 400 MPa/25°C/5 min and T3: 600 MPa/25°C/5 min (treatments). In addition, the difference among diced, freeze-dried and pulverized onions (groups) was studied, in order to select the process more adequate for better preserving volatile compounds. The results obtained in full scan mode showed that both main factors (group and treatment) had a significant effect ($P<0.001$). There were also significant differences between groups and treatments for all compounds, being the main effect of group more marked by HS GC-MS using selective ion monitoring (SIM) mode. For 2-methyl 2-pentenal, dimethyl trisulfide, and methyl propyl trisulfide it has been observed an increase in freeze-dried and pulverized onion samples compared with diced samples regardless the HP treatment. However, freeze-drying and pulverization processes affected the stability of propionaldehyde, 1-propanethiol, hexanal, dipropyl disulfide, and dipropyl trisulfide, diminishing their content regardless the HP treatment. HP at 200 and 400 MPa/25°C/5 min were the least detrimental treatments to the total fraction of volatile compounds, not affecting or even increasing the levels of some volatile compounds. Onion is widely used worldwide in various forms for both food and medicinal applications, thanks to its high content of phytonutrients, such as flavonoids and volatile sulfur compounds. Fresh onion is very perishable and drying is widely applied for extending shelf-life, thus obtaining a very easy-to-use functional food ingredient. The flavonoid and volatile fractions of different onion cuts (flakes, rings) prepared through different drying cycles in a static oven, were characterized by high-performance liquid chromatography with a diode-array detector HPLC-DAD, Head Space-Solid Phase Micro Extraction followed by Gas Chromatography coupled with Mass Spectrometry (HS-SPME-GC-MS) and Head-Space Solid Phase Micro Extraction followed by comprehensive two-dimensional Gas-Chromatography (HS-SPME-GC×GC-TOF). Onion flakes showed a significantly higher flavonoid content (3.56 mg g^{-1}) than onion rings (2.04 mg g^{-1}). Onion flakes showed greater amount of volatile organic compounds (VOCs) (127.26 mg g^{-1}) than onion rings (42.79 mg g^{-1}), with different relative amounts of di- and trisulfides-disulfides largely predominate the volatile fraction (amounts over 60% on the total volatile content), followed by trisulfides and dipropyl disulfide and dipropyl trisulfide were the most abundant VOCs. HS-SPME-GC×GC-TOF allowed for the detection of the presence of allylthiol, diethanol sulfide, 4,6-diethyl1,2,3,5-tetrathiolane, not detected by HS-SPME-GC-MS, and provided a fast and direct visualization and comparison of different samples. These results highlight different nutraceutical properties of dried onion samples processed otherwise, only differing in shape and size, thus pointing out potentially different uses as functional ingredients.

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Biography

Chong Mun Hwa has completed her PhD from University Teknologi Malaysia and has more than 7 years of experience in analytical field. She is currently the Senior Analytical Chemist of Synthomer, an aqueous polymer organization. She has published paper in Microporous and Mesoporous Materials journal, a co-author for the book chapter membrane-based solid phase extraction (UTM), had 1 patent for method of extracting chemicals (nitrosamines) in water

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