

Editorial note on Chemical Diversity and Complexity of Scotch Whisky

Suresh Babu G

Department of Biotechnology, Rvr & Jc College of Engineering, Guntur, Andhra Pradesh, India.

Editorial Note

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For Correspondence

Suresh Babu G, Department of biotechnology, Rvr & Jc college of Engineering, Guntur, AP, India.

E-mail: gogineni1988@gmail.com

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EDITORIAL NOTE

Scotch whisky, both traditionally and commercially, is a significant commodity. Chemically, Scotch Whisky is a complex combination composed of thousands of ingredients, the origin of which is largely unclear. Here, as observed by Fourier transform ion cyclotron resonance mass spectrometry, we give a detailed description of Scotch Whisky's chemistry (FT-ICR MS). Eighty-five whiskies were analysed by untargeted high-resolution mass spectrometry, comprising majority of the Scotch whisky produced and sold. For each sample, thousands of chemical formulas were allocated based on the parts-per-billion mass precision of FT-ICR MS spectra. Isotopic fine structure analysis was used for the first time to validate the assignment of CHOS species of high molecular weight in Scotch Whisky. A variety of visualization methods, including van Krevelen diagrams, double bond equivalence (DBE) maps, as well as heteroatomic compound type distributions, were used to compare the given spectra. In addition, multivariate analysis was used to analyze the results, like PCA and OPLS-DA, with main compounds defined for distinguishing between types of whisky (blend or malt) or wood type maturation. Scotch Whisky's FT-ICR MS research has been shown to have considerable potential to better explain the complexity of mature spirit drinks and as a method for analyzing the chemistry of maturation processes.

Scotch Whisky, both economically and traditionally, is a high-value commodity, producing £ 3.86bn in UK exports to over 200 countries in 2015. Chemically speaking, Scotch Whisky is a complex combination of several thousand substances of a relatively unknown origin. Such dynamic mixtures, such as soil organic matter, dissolved organic matter, or organic aerosols, can be compared from this point of view. In the development of methods for its characterization at the molecular level, natural organic matter (NOM) is the focus of extensive study. Studies of metabolites, plant extracts, or, even, other foods or liquids are linked to these efforts. Thus, this dissertation leads to reaching larger analytical chemistry targets in the field of complex mixture analysis.

Scotch Whisky's routine research requires separation methods, such as gas or liquid chromatography, often combined with widely available detectors, including UV, flame ionization (FID) or mass spectrometry detectors (MS). Many of the main compounds in whisky have been characterized by these processes. This analysis are extremely targeted, and particular congeners' determined concentrations are also used as a test of whisky's authenticity. The amounts of 2- and 3-methyl-butanol, for example, are related to the relative amount of malt in a mixed whisky drink. This type of targeted strategy is very beneficial, but it has its limitations.

The chemical complexity of Scotch Whisky has been uncovered by high-resolution mass spectrometry, allowing thousands of compounds to be detected, rather than hundreds, as commonly associated with this substance. As shown by the contrast of mature samples to a new-make spirit, we prove that this difficulty emerges by cask-maturation. The specific chemical processes that occur during maturation remain unclear, but the findings obtained here provide a roadmap to gaining an understanding of the chemistry of maturation. Potential chemical indicators, including those representing the varieties of maturing timber, have been discovered for processing methods. The nature of many of the formulae found remains unknown, and future studies will research time series of maturation cask samples to better explain maturation processes, including their kinetics. FT-ICR MS has been proven to be a powerful tool for Scotch Whisky research, and this approach may be of considerable use in researching other mature spirit drinks and other complex drinks.