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WHITE PAPER

AUTOMATED FOOD-FLAVOR ANALYSIS USING SIFT-MS

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ABSTRACT

Aroma compounds have diverse chemical functionalities, impart a wide range of favorable and unfavorable sensations to the human olfactory system, and have a wide range of sensory thresholds. Conventional analytical technologies (based, for example, on gas chromatography) lack the combined time resolution and comprehensiveness of analysis required to provide rapid feedback for product developers, quality managers, and process-line operations. Selected ion flow tube mass spectrometry (SIFT-MS) is a start-of-the-art, direct-analysis technology for rapid, high sensitivity, high specificity, and robust analysis of aroma compounds in air and headspace at trace concentrations. In its automated form, SIFT-MS is readily applied to diverse high-throughput food analysis applications, including objective sensory analysis, authentication, and ingredient screening.

THE SIGNIFICANCE OF VOLATILE COMPOUNDS IN FOOD AND THEIR ANALYSIS

Detection of volatile organic compounds (VOCs) is vitally important in the food and flavor industry for several reasons. For example, they can function individually as markers of food quality and freshness, and together as an overall volatile "fingerprint" that can enable determination of product origin or differentiate between commercial products, for example. Furthermore, these VOCs can play a major part in aroma sensory experience.

Analysis of aroma compounds in both quality assurance and new product development applications benefits significantly from analysis of larger sample numbers to support effective decision making. However, traditional analytical technologies used for VOC analysis – most notably gas chromatography-mass spectrometry (GC-MS) – are poorly equipped to address these needs. Factors that preclude high-throughput and real-time analysis using GC-MS include:

- **Chromatographic separation involves separating analytes in time**, leading to extended analysis times.
- **Chromatographic columns are discriminatory**, so these approaches cannot provide a complete analysis of chemically diverse aroma compounds in the sample, which is especially important for sensory applications.
- Achieving **low detection limits** (part-per-billion-by-volume (ppbV) and below) that are typical for the human olfactory system usually requires preconcentration.
- **Removal of moisture** prior to analysis.

Selected ion flow tube mass spectrometry (SIFT-MS) addresses and resolves these shortcomings, providing robust high-throughput and high-time-resolution VOC analysis with simplicity and flexibility. This whitepaper describes the application of automated SIFT-MS to high-throughput:

- Product quality and sensory-correlated analysis,
- Origin, varietal, and authentication screening, and
- Product identification and matching.

These diverse applications – and more – can be achieved using a single automated SIFT-MS instrument, supporting highly efficient use of analytical instrumentation.

SELECTED ION FLOW TUBE MASS SPECTROMETRY (SIFT-MS) – A BRIEF INTRODUCTION

SIFT-MS is the leading real-time analytical technique for comprehensive gas and headspace analysis to ultra-trace concentrations. SIFT-MS (Figure 1) uses ultra-soft, precisely controlled chemical ionization (CI) coupled with mass spectrometric detection to rapidly quantify VOCs and permanent gases to sub-part-per-billion concentrations by volume (ppbV). Up to standard eight chemical ionization agents (reagent ions) are available in Syft Technologies SIFT-MS instruments, such as the Syft Tracer™: H_3O^+, NO^+, $O_2^{+\cdot}$, OH^-, $O^{-\cdot}$, $O_2^{-\cdot}$, NO_2^-, and NO_3^-. These reagent ions react with analyte VOCs and inorganic gases in very well controlled ion-molecule reactions, but they have very slow or no reaction with the major components of air (N_2, O_2, Ar, CO_2 and H_2O). This enables SIFT-MS to analyze air at trace and ultra-trace levels without preconcentration or sample drying. Rapid switching of reagent ions provides unsurpassed specificity compared to other direct-analysis techniques. To learn more about SIFT-MS, see the Technology Overview (https://syft.com/assets/Knowledge-Centre/SIFT-MS-Overview_Mar-2023.pdf) and recent review articles (Langford (2023) and Smith *et al*. (2023)).

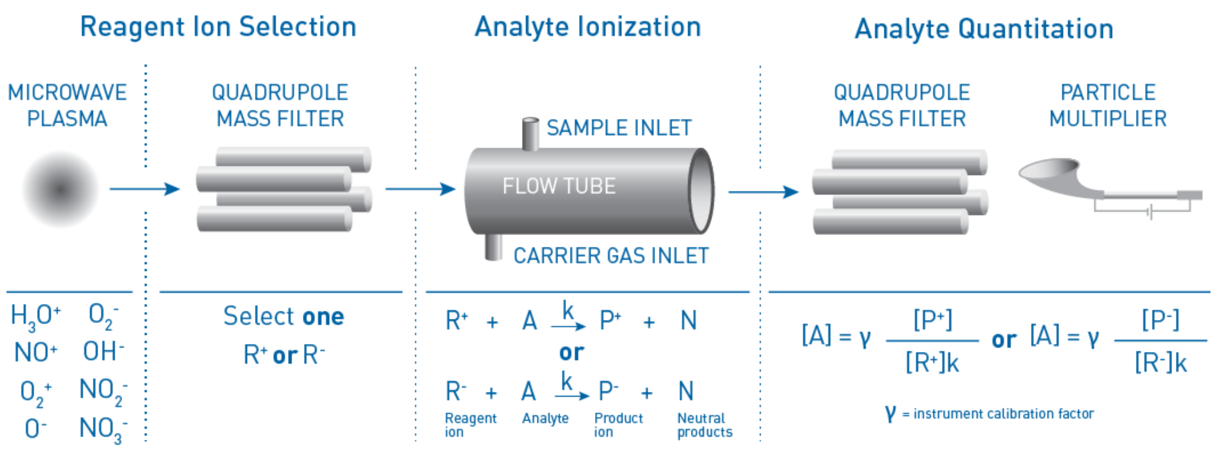


Figure 1. Schematic representation of the SIFT-MS technique.

1. Automation of SIFT-MS Instruments

Automated-SIFT-MS analysis is readily achieved using ‘xyz’ robotic autosamplers from CTC Analytics and Gerstel that utilize syringe-based sample injection (Langford and Perkins (2024)). Various headspace approaches are compatible with automated SIFT-MS instruments, including static headspace analysis (SHA), the method of standard additions (MoSA), and multiple headspace extraction (MHE). Advanced SIFT-MS and autosampler software enable extremely efficient workflows to be achieved through optimized sample scheduling (Langford and Perkins (2024)).

2. Targeted and Untargeted Approaches

SIFT-MS can be utilized for both targeted (selected ion monitoring, SIM) and untargeted (full scan) analysis, each with distinct benefits. SIM mode enables direct, quantitative analysis of targeted aroma compounds, whereas full-scan mode provides a broader view of the sample and can be used to detect volatiles that are outside a target compound suite – albeit with a modest reduction in sensitivity and response time. Using full-scan mode with multivariate statistical analysis enables mass spectral “fingerprinting” to be conducted, supporting aroma quality control workflows, etc. (Langford and Perkins (2023)).

3. Multivariate Statistical Analysis of SIFT-MS Data

Many food products have a complex VOC profile. To simplify differentiation of samples with varying characteristics and accommodate correlation with human sensory perception, multivariate statistical analysis is often applied to SIFT-MS data. Soft independent modeling by class analogy (SIMCA) (Wold (1976)) – an enhanced form of principal component analysis (PCA) – has been most widely utilized (Langford *et al.* (2019)), although other statistical approaches can also be used (Viaene and vander Heyden (2018)). The SIMCA interclass distance metric used to assess the ability of SIFT-MS to distinguish between pre-defined sample classes and should have a value greater than three (Kvalheim and Karstang (1992)).

PRODUCT QUALITY AND SENSORY-CORRELATED ANALYSIS

Product quality, which impacts food safety and sensory experience in terms of volatiles, is a very important consideration for food manufacturers. Human sensory analysis benchmarks consumer acceptance of food and fragrance products, but it is expensive, subject to fatigue, and has been very difficult to conduct on the process line. With sensitive, broad-spectrum, and rapid analysis, SIFT-MS is an effective technique for both real-time and high-throughput quality analysis.

Depending on the complexity of the aroma, there are several possible approaches for instrument-based assessment of product quality. Three approaches are illustrated below.

1. Edible Oil Oxidation

First, for systems with a relatively simple headspace, quantitation of quality markers versus simple concentration thresholds is a straightforward approach. For example, determination of the extent of edible oil oxidation can be achieved by targeting VOCs – primarily saturated and unsaturated aldehydes – that are indicative of lipid oxidation. Detection of edible oil oxidation is achieved easily by applying SIFT-MS to instantaneous quantitation of volatile markers. Figure 2(a) shows quantitation of propanal in the headspace of fish oil as it oxidizes over several days (Syft Technologies (2016)). Acetaldehyde, acetone, hexanal and ethanol showed very similar trends (Figure 2(b)). Analysis of each sample takes less than one minute, supporting high-throughput screening – whether of ingredients or finished products. Furthermore, the high sensitivity of SIFT-MS analysis enables oxidation products to be detected early.

2. Parmesan Cheese

SIFT-MS can also be used to target dominant odor-active volatiles (OAVs) in a food product. This approach was first utilized with SIFT-MS in a 2012 study comparing four genuine Italian and four imitation New Zealand Parmesan cheeses (Langford *et al.* (2012a)). Discrimination of the individual products, in addition to more general origin determination, was achieved based on OAVs. Subsequent work using automated headspace analysis (Perkins *et al.* (2021a)) demonstrated improved repeatability compared to the earlier manual headspace work. Retail products from several Italian manufacturers were differentiated (Figure 3), since all interclass distances were greater than three.

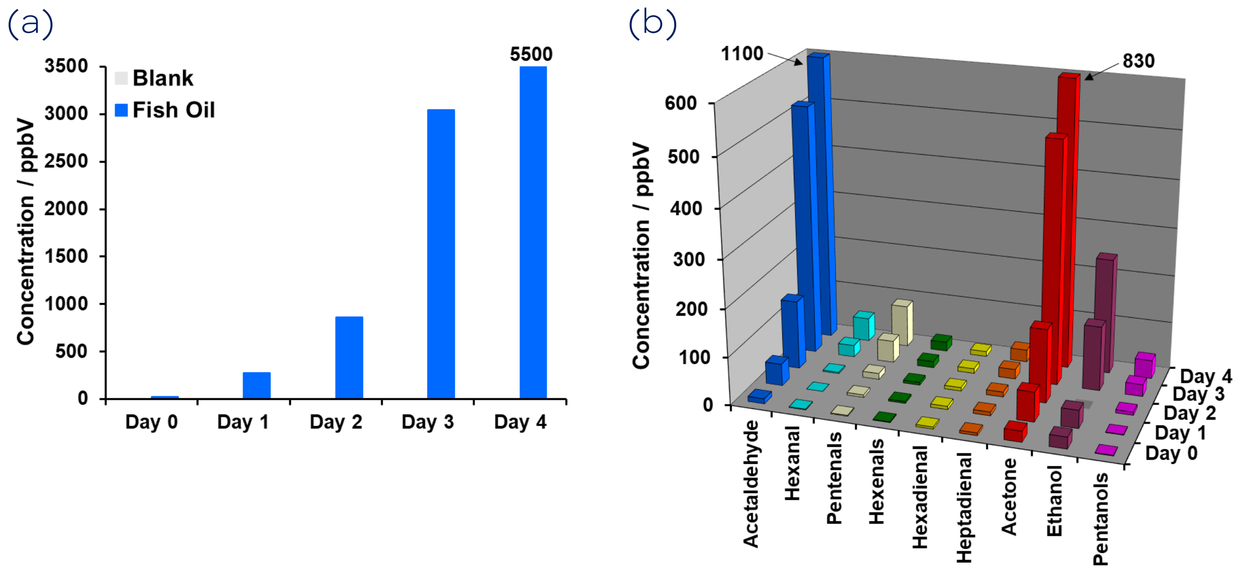
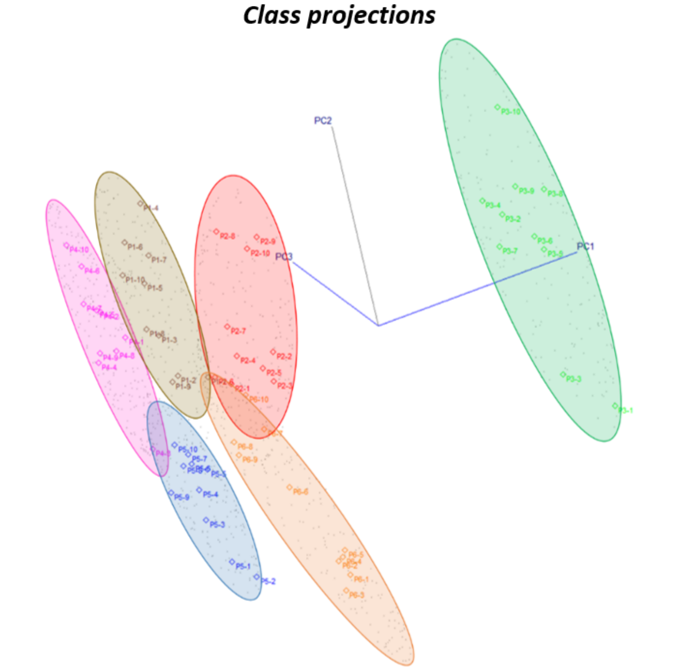


Figure 2. Oxidation of fish oil over several days monitored using headspace-SIFT-MS analysis: (a) propanal and (b) other oxidation/degradation markers.

Class projections



Discriminating power

Odor-active compound	DP
Acetaldehyde	116193
Methylbutanal isomers	4382
Phenylacetaldehyde	4293
Butanoic acid	3048
Ethyl butanoate	2322
Dimethyl trisulfide	2071
Hexanal	1772
2-Methylpropanal	1227
Ethyl octanoate	1014
Acetic acid	994
Hexanoic acid	967
2,3-Butanedione	817
2,3-Dimethylpyrazine	685
Methional	113
Ethyl hexanoate	86

Interclass distances

Product	P2	P3	P4	P5	P6
P1	4.7	35.1	33.1	13.3	4.8
P2		18.1	23.8	8.7	3.0
P3			172	58.2	20.7
P4				5.1	41.1
P5					13.8

Figure 3. Classification of genuine Italian Parmesan cheeses by individual retail products using automated headspace-SIFT-MS analysis to target odor-active volatiles (Perkins et al. (2021a)). SIMCA class projections, interclass distances, and discriminating powers of the 15 odor-impact compounds are shown.

3. Beef Aroma Quality

The most comprehensive approach to correlating SIFT-MS measurements with those obtained by a human sensory panel involves combining data from both sources using multivariate statistical analysis. This approach enables the creation of a model that correlates the SIFT-MS data with the product classification according to odor descriptor assigned by the panelists. The model can then be utilized to predict sensory panel results based on SIFT-MS measurements.

Figure 4 shows SIFT-MS concentration data for beef samples that have prime and defective (eight) beef aromas, as judged by a trained sensory panel (Langford *et al.* (2018)). Combining sensory data with measurements from SIFT-MS, multivariate statistical analysis using SIMCA enables differentiation of all sensory classes instrumentally (Figure 5). Hence SIFT-MS can rapidly grade beef aroma quality from sample VOC profiles, providing an objective, rapid sensory test that enables many more samples to be graded per day than a traditional sensory panel.

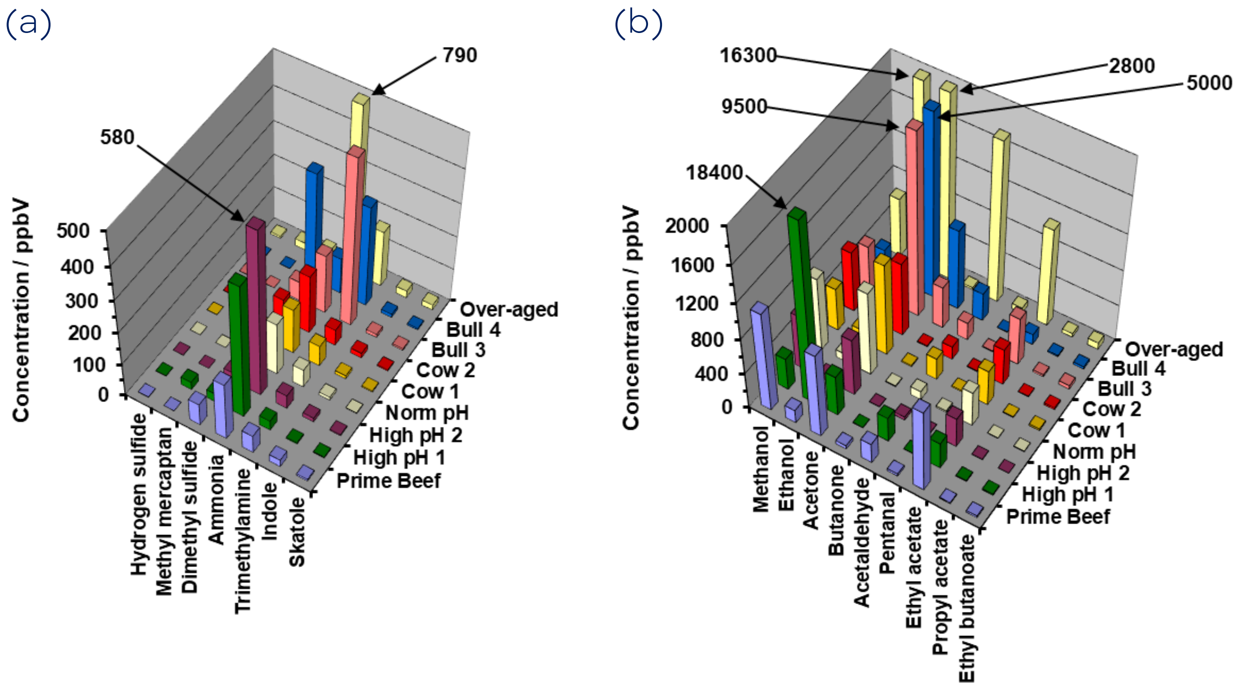


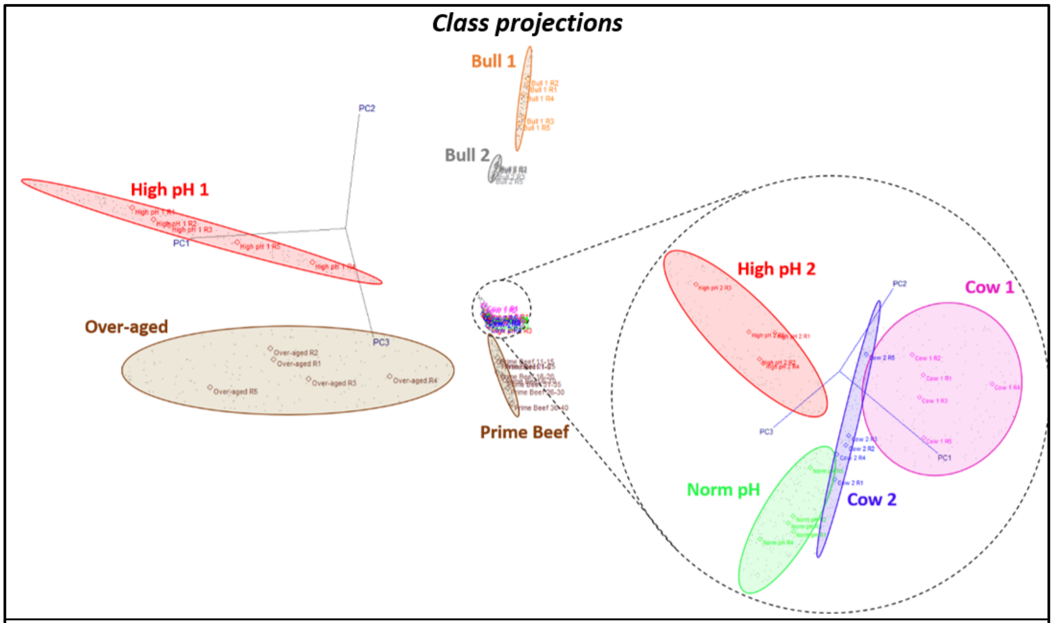
Figure 4. Headspace-SIFT-MS concentrations of (a) oxygenates and (b) sulfur- and nitrogen-containing compounds, obtained for beef samples classified according to their sensory descriptor (Langford et al. (2018)). Note that the SIFT-MS method collected data for all analytes in one analysis.

ORIGIN, VARIETAL, AND AUTHENTICITY DETERMINATION

For certain food products or ingredients, volatile compound profiles can be used to screen for origin and/or variety, as illustrated in this section.

1. Coffee Bean Origin

Coffee beans have distinct regional aroma variations arising from different relative concentrations of volatiles. SIFT-MS has potential to be utilized for confirmation of origin both for single-origin coffee products and for quality assessment of blends.



Interclass distances

Sensory descriptor	High pH 2	Norm pH	Cow 1	Cow 2	Bull 1	Bull 2	Over-aged	High pH 1
Prime beef	15	8.2	8.5	7.0	51	35	56	174
High pH 2		14	5.6	7.3	57	41	60	226
Norm pH			4.1	4.3	30	32	57	226
Cow 1				3.3	45	26	56	166
Cow 2					64	43	55	191
Bull 1						26	61	216
Bull 2							58	210
Over-aged								13

Figure 5. SIFT-MS classification of prime and defective beef samples using SIMCA multivariate statistical analysis of the headspace concentration data (Langford et al. (2018)). The cluttered region of the class projection plot is expanded on the right (indicated in the interclass distances by grey cell shading). The pink-shaded interclass distances highlight the separation between premium and defective samples.

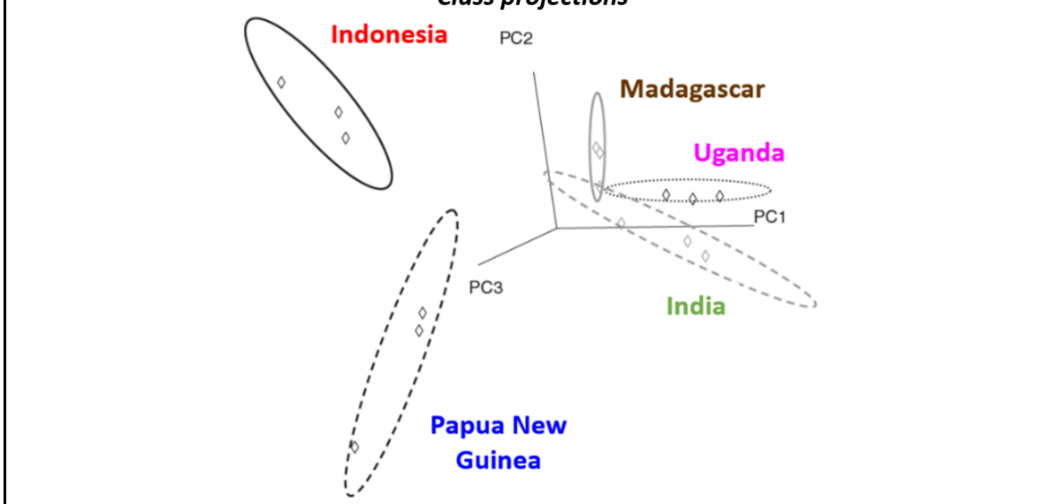
Green coffee beans of five origins – Brazil, Colombia, Ethiopia, Guatemala, and Sumatra – were analyzed using automated headspace-SIFT-MS (Syft Technologies (2017)). Multivariate statistical analysis using the SIMCA algorithm yielded the interclass distances shown in Table 1, indicating that all coffee origins can be distinguished. Dryahina *et al.* (2018) have also demonstrated that SIFT-MS combined with PCA can classify by origin after roasting.

Country of Origin	Colombia	Ethiopia	Guatemala	Sumatra
Brazil	7.7	5.9	5.5	13
Colombia		8.5	17	6.0
Ethiopia			4.0	15
Guatemala				34

Table 1. Interclass distances from SIMCA analysis of the green coffee concentration data obtained using SIFT-MS.

2. Vanilla Extract Origin

Vanilla extracts from India, Indonesia, Madagascar, Papua New Guinea, and Uganda, supplied by a well-known United States ingredient brand, were distinguished using SIFT-MS headspace analysis and SIMCA multivariate statistical analysis (Sharp *et al.* (2012); Figure 6). Due to the ethanol carrier solvent in these extracts, samples were placed on filter paper, the ethanol evaporated, and then the filter paper was equilibrated in headspace bottles for one hour prior to the 90-s SIFT-MS analysis. Vanillin, anise alcohol, and 4-methylguaiacol were the three most significant volatiles contributing to differentiation of the extracts.



Interclass distances

Origin	Uganda	India	Madagascar	Papua New Guinea
India	4.5	11	23	29
Uganda		6.2	20	30
Madagascar			16	18
Indonesia				8.3

Figure 6. Discrimination of vanilla extract origins using SIFT-MS with SIMCA multivariate statistical analysis. SIMCA class projections and interclass distances are shown.

3. High Value Natural Edible and Cosmetic Oils

High-value oils, such as Argan oil and olive oil, are vulnerable to fraudulent activities, including falsified origin labeling and adulteration. Hence assuring their integrity is important to genuine producers.

Vercammen and co-workers pioneered both untargeted SIFT-MS food analysis in the literature and demonstrated that the approach could be utilized for high-throughput origin authentication of high-value Argan and olive oils (Kharbach *et al.* (2018), Bajoub *et al.* (2018)). Using this approach, they subsequently demonstrated adulteration detection in Argan oil (Kharbach *et al.* (2022)). Ozcan-Sinir (2020) demonstrated that adulteration of olive oil by commodity edible oils (corn and sunflower) is detectable using SIFT-MS combined with multivariate statistical analysis.

4. Honey

Honeys have diverse aroma characteristics depending on the nectar source. Langford *et al.* (2012b) analyzed headspace volatiles from nine monofloral New Zealand honeys and were able to differentiate them on this basis. Similarly, Agila and Barringer (2012) investigated monofloral North American honeys using SIFT-MS to determine the influence of location and plant species. These researchers also studied the effect of high fructose corn syrup adulteration (at 5% to 40%) on five honeys (blueberry, star thistle, clover, wildflower, and an unknown source to simulate honey adulteration). The volatile profiles determined using SIFT-MS showed significant differences for adulterated honeys (Agila and Barringer (2013)).

PRODUCT IDENTIFICATION AND MATCHING

The sensitive and broad-spectrum aroma compound detection provided by SIFT-MS confers the ability to rapidly identify and match products. This can be achieved using targeted and untargeted approaches. Here, untargeted analysis is illustrated using two examples: beer and strawberry flavor mixes.

1. Beer

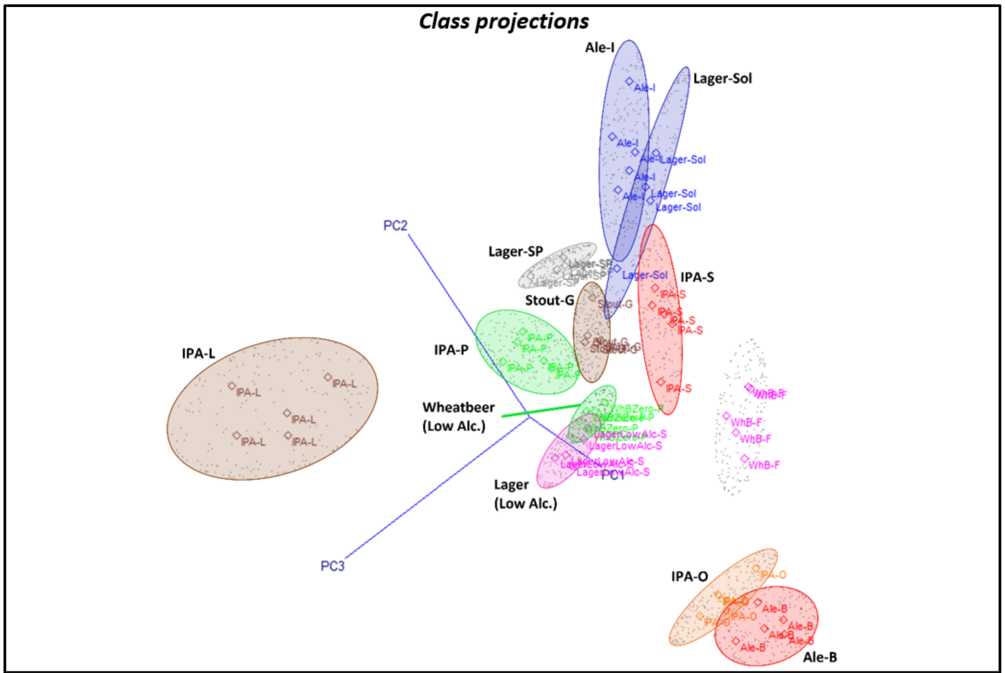
Beer, with typical alcohol levels of 5 to 7%, is readily analyzed using automated headspace-SIFT-MS following 10-fold dilution in water, coupled with typically 10-fold dilution of headspace in make-up gas during injection into the instrument inlet (Langford and Perkins (2024)). Figure 7 shows the results obtained from applying SIMCA data processing to full-scan SIFT-MS data (H_3O^+ reagent ion) obtained for 12 beer products (Perkins *et al.* (2021b)). The interclass distances demonstrate that all products are distinguished using SIFT-MS.

2. Strawberry Flavor Mixes

A similar analytical approach has been utilized for classification of commercial strawberry flavor mixes for batch-to-batch and inter-mix variations (Langford and Bell (2019)) – demonstrating potential for flavor matching. In this study, three anonymized flavor mixes were supplied for SIFT-MS evaluation versus two labelled formulations (three batches of each). Five replicates were prepared for each sample type/batch. The results obtained following SIMCA processing of the SIFT-MS full-scan data (NO^+ reagent ion) are summarized in Figure 8. As highlighted by the interclass distances (and confirmed visually in the class projections):

- **Unknown 1 (U1)** is a fourth batch of flavor standard 1 (S1). Although the interclass distance between U1 and S1 is >3, the three batches (identified as S1a, S1b, and S1c) were all readily differentiable based on their volatile profiles due to significant batch-to-batch variability.
- **Unknown 2 (U2)** is another batch of flavor standard 2 (S2), because the interclass distance is very small.
- **Unknown 3 (U3)** differs from all other flavor mixes, as indicated by large interclass distances with all other samples. It represents a completely different (i.e., a third) formulation.

This study demonstrates that SIFT-MS can be utilized to identify products or ingredients, confirm the integrity of products or ingredients, and – by extension – provide rapid assessment of similarity in aroma matching.

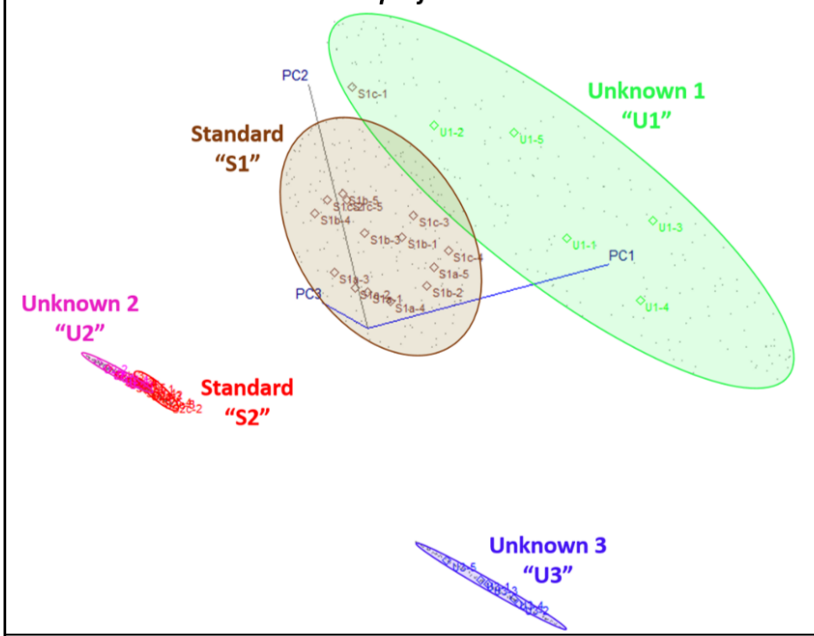


Interclass distances

Product	Ale-B	IPA-P	Wheat beer-F	Ale-I	IPA-O	Lager-SP	IPA-L	IPA-S	Wheat beer (Low Alc.)	Lager (Low Alc.)	Lager-Sol
Stout-G	36.3	7.8	18.4	17.1	15.4	12.2	6.5	3.6	17.2	25.1	5.5
Ale-B		10.0	4.9	26.6	8.0	35.9	15.5	15.8	47.9	61.9	33.9
IPA-P			5.8	5.1	7.3	7.7	4.3	5.5	20.9	20.4	7.0
Wheat beer-F				11.4	5.6	18.5	11.5	11.5	32.0	31.7	16.8
Ale-I					14.5	17.6	6.8	6.7	35.0	56.9	10.6
IPA-O						17.0	10.7	8.5	27.3	27.4	17.2
Lager-SP							5.9	3.8	24.4	36.9	9.2
IPA-L								5.3	16.1	14.7	6.7
IPA-S									15.3	13.9	3.9
Wheat beer (Low Alc.)										5.6	21.7
Lager (Low Alc.)											29.0

Figure 7. Classification of 12 beer products (Perkins et al. (2021b)) using untargeted SIFT-MS analysis (H_3O^+ reagent ion) coupled with SIMCA multivariate statistical analysis. Class projections and interclass distances are shown. Note: IPA is India pale ale.

Class projections



Interclass distances

Sample Code	S2	U1	U2	U3
S1	33.6	3.5	63.0	58.5
S2		23.6	0.91	18.1
U1			47.9	46.5
U2				19.3

Discriminating power

m/z	DP
75	55600
225	5040
152	4440
81	4330
141	4070
200	2950
197	2870
114	2280
204	2190
110	2130

Figure 8. Classification of unidentified strawberry flavor mix samples (U1, U2, and U3) as flavor standard S1 or S2, or neither. Class projections, interclass distances, and the most significant 10 variables (mass-to-charge ratios; m/z) for discrimination of the samples are shown. Interclass distances shaded in gray are discussed in the text.

CONCLUSIONS

In a single platform, automated SIFT-MS instruments empower both new product development and routine testing laboratories by providing:

- Simple, fast freshness and quality screening,
- Raw material origin and varietal authentication,
- High-throughput, objective sensory analysis, and
- The ability to differentiate, identify, and match products.

Through rapid, sensitive, and comprehensive analysis, automated SIFT-MS instruments provide new opportunities for aroma analysis at very low cost per sample.

REFERENCES

Agila A, Barringer, S (2012). Application of selected ion flow tube mass spectrometry coupled with chemometrics to study the effect of location and botanical origin on volatile profile of unifloral American honeys. *J. Food Sci.* 77, C1103-C1108. https://doi.org/10.1111/j.1750-3841.2012.02916.x

Agila A, Barringer S (2013). Effect of adulteration on volatiles in unifloral honeys from different floral sources and locations. *J. Food Sci.* 78, C184-C191. https://doi.org/10.1111/1750-3841.12033

Bajoub A, Medina-Rodriguez S, Ajal EA, Cuadros-Rodríguez L, Monasterio RP, Vercammen J, Fernández-Gutiérreza A, Carrasco-Pancorbo A (2018). A Metabolic Fingerprinting Approach Based on [SIFT-MS] and Chemometrics: A Reliable Tool for Mediterranean Origin-Labelled Olive Oils Authentication. *Food Res. Int*. 106, 233–242. https://doi.org/10.1016/j.foodres.2017.12.027

Dryahina K, Smith D, Španěl P (2018). Quantification of volatile compounds released by roasted coffee by selected ion flow tube mass spectrometry. *Rapid Commun Mass Spectrom*. 32, 739-750. https://doi.org/10.1002/rcm.8095

Kharbach M, Kamal R, Mansouri AM, Marmouzi I, Viaene J, Cherrah Y, Alaoui K, Vercammen J, Bouklouze A, Vander Heyden Y (2018). [SIFT-MS] Fingerprinting Versus Chemical Profiling for Geographic Traceability of Moroccan Argan Oils. *Food Chem*. 263, 8–17. https://doi.org/10.1016/j.foodchem.2018.04.059

Kharbach M, Yu HW, Kamal R, Marmouzi I, Alaoui K, Vercammen J, Bouklouze A, Vander Heyden Y (2022). Authentication of Extra Virgin Argan Oil by [SIFT-MS] fingerprinting and chemometrics. *Food Chem.* 383, 132565. https://doi.org/10.1016/j.foodchem.2022.132565

Kvalheim OM, Karstang TV (1992). SIMCA - classification by means of disjoint cross validated principal components models. In *Multivariate Pattern Recognition in Chemometrics, Illustrated by Case Studies*. Brereton RG, Ed. Elsevier: Amsterdam; 209-238.

Langford VS (2023). SIFT-MS: Quantifying the volatiles you smell . . . and the toxics you don't. *Chemosensors* 11, 111. https://doi.org/10.3390/chemosensors1102011

Langford VS, Bell KJM (2019). Rapid Determination of Strawberry Flavour Integrity Using Static Headspace-[SIFT-MS]. *Chromatogr. Today* **2019**, *12*(3), 2-6. https://www.chromatographytoday.com/article/gc-ms/46/syft-technologies-ltd/rapid-determination-of-strawberry-flavour-integrity-using-static-headspace-selected-ion-flow-tube-mass-spectrometry/2558/download

Langford VS, Gray J, Foulkes B, Bray P, McEwan MJ (2012b). Application of selected ion flow tube- mass spectrometry to the characterization of monofloral New Zealand honeys. *J. Agric. Food Chem.* 60, 6806-6815. https://doi.org/10.1021/jf3025002

Langford VS, McEwan MJ, Cummings T, Simmons N, Daly C (2018). Rapid classification of beef aroma quality using SIFT-MS. *Adv. Food Bev. Anal.* (Supplement to *LCGC North America*). 1, 8-15. https://www.chromatographyonline.com/view/rapid-classification-beef-aroma-quality-using-sift-ms

Langford VS, Padayachee D, McEwan MJ, Barringer SA (2019). Comprehensive odorant analysis for on-line applications using [SIFT-MS]. *Flavour Fragr. J.* 34, 393-410. https://doi.org/10.1002/ffj.3516

Langford VS, Perkins MJ (2023). Rapid untargeted screening of food and ingredient aroma using direct-injection mass spectrometry. *Column*, *19*(6), 23-26. www.chromatographyonline.com/view/rapid-untargeted-screening-of-food-and-ingredient-aroma-using-direct-injection-mass-spectrometry

Langford VS, Perkins MJ (2024). Improved volatiles analysis workflows using automated [SIFT-MS]. ***Anal. Methods*** 16, 8119-8138. https://doi.org/10.1039/D4AY01707B

Langford VS, Reed CJ, Milligan DB, McEwan MJ, Barringer SA, Harper (2012a)**. Headspace analysis of Italian and New Zealand Parmesan cheeses.** *J. Food Sci.* **77, C719**-C726. https://doi.org/10.1111/j.1750-3841.2012.02730.x

Ozcan-Sinir, G (2020). Detection of adulteration in extra virgin olive oil by [SIFT-MS] and chemometrics. *Food Control* 118, 107433. https://doi.org/10.1016/j.foodcont.2020.107433

Perkins MJ, Padayachee D, Langford VS (2021a). Rapid Parmesan classification using automated static headspace-SIFT-MS analysis. Syft Technologies Application Note. https://bit.ly/4d7zXAi

Perkins MJ, Padayachee D, Langford VS (2021b). Rapid classification of beer using untargeted SIFT-MS headspace analysis. Syft Technologies Application Note. http://bit.ly/40n3LT4

Sharp MD, Kocaoglu-Vurma NA, Langford V, Rodriguez-Saona LE, Harper WJ (2012). Rapid discrimination and characterization of vanilla bean extracts by attenuated total reflection infrared spectroscopy and [SIFT-MS]. *J. Food Sci.* 77, C284-C292. https://doi.org/10.1111/j.1750-3841.2011.02544.x

Smith D, Španěl P, Demarais N, Langford VS, McEwan MJ (2023). Recent developments and applications of [SIFT-MS]. *Mass Spec. Rev.* e21835. https://doi.org/10.1002/mas.21835

Syft Technologies (2016). Simple, instant detection of fish oil oxidation. Syft Technologies Application Note. https://bit.ly/4lQJK2B

Syft Technologies (2017). Rapid determination of coffee origin. Syft Technologies Application Note. https://bit.ly/4jJm7HF

Viaene J, vander Heyden Y (2018). Introduction to herbal fingerprinting by chromatography. In *Chemometrics in Chromatography*. Komsta Ł, Heyden YV, Sherma J, Eds. Boca Raton: CRC Press; 506 p.

Wold S (1976). Pattern recognition by means of disjoint principal components models, *Pattern Recognition*, 8, 127-139.

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