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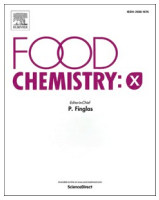

Comparative study on chemical compositions and volatile profiles of seed oils from five common Cucurbitaceae species

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ABSTRACT

The chemical compositions and volatile profiles of wax gourd seed oil (WGSO), watermelon seed oil (WSO), pumpkin seed oil (PSO), cucumber seed oil (CSO), and bitter gourd seed oil (BGSO) were comparatively explored for the first time. All oils complied with standards for physicochemical properties and BGSO had the highest phenolic content. Their mineral levels varied significantly. The fatty acid composition of WGSO, WSO, PSO, and CSO was similar, predominantly linoleic acid. Whereas BGSO exhibited a distinct fatty acid profile with 55.38 % α-eleostearic acid. All samples were rich in tocopherols and squalene, with WSO having the highest total tocopherol content and PSO having the highest squalene content. HS-GC–IMS and HS-SPME-GC–MS detected 118 and 67 VOCs, respectively, primarily consisting of aliphatic aldehydes, alcohols, esters, and ketones. Principal component analysis confirmed that BGSO had the most distinctive volatile characteristics, while the other four seed oils shared similar VOC profiles.

1. Introduction

The seeds of Cucurbitaceae fruits, such as wax gourd (*Benincasa hispida*), pumpkin (*Cucurbita moschata*), watermelon (*Citrullus lanatus*), cucumber (*Cucumis sativus* L.), and bitter gourd (*Momordica charantia*), are commonly consumed as snacks after roasting or salting in East Asia and Arab countries, owing to their high lipid and protein content (Murthy et al., 2022; Yao et al., 2019). Over the past decades, Cucurbitaceae seed oils have gained attention for their high levels of polyunsaturated fatty acids and bioactive compounds (Yoshime et al., 2019). Pumpkin seed oil (PSO), watermelon seed oil (WSO), wax gourd seed oil (WGSO), and cucumber seed oil (CSO) have similar fatty acid profiles dominated by linoleic acid (C18:2), which accounts for 47.32 %, 72.45 %, 76.77 %, and 65.71 % of the total fatty acid compositions, respectively (Murthy et al., 2022; Yao et al., 2019). The relatively lower linoleic acid content in PSO is attributed to its high oleic acid percentage (C18:1) (Nawirska-Olszańska et al., 2013). Additionally, WGSO has the highest tocopherol content among them, while PSO contains a notable squalene content of 2732 mg/kg (Murthy et al., 2022; Yao et al., 2019). Bitter gourd stands out as one of the few edible fruits that contain a rich amount of conjugated α-linolenic acid. The bitter gourd seed oil (BGSO) is comprised of 30–60 % α-eleostearic acid, which is associated with potential health benefits such as antioxidant, anti-atherosclerotic, and antitumor properties (Yoshime et al., 2016). However, most current publications focuses on the fatty acid compositions or antioxidant abilities of PSO or WSO (Nawirska-Olszańska et al., 2013; Yao et al., 2019), and there is a lack of comparative studies on the chemical compositions of these Cucurbitaceae seed oils.

Volatile organic compounds (VOCs) are key factors that impact food flavor quality and consumer preference. The VOCs of edible oils are diverse, mainly comprising aldehydes, ketones, acids, esters, alcohols, phenols, and heterocyclic compounds (Zhang et al., 2021). These components primarily formed from fatty acids and amino acids, vary significantly based on factors such as oil crop varieties, process conditions, and the geographical origin of plants (Sun et al., 2023). Thus, revealing the volatile profiles in different edible oil varieties not only aids in discerning the aroma features but also provides a volatile reference for quality control of edible oil products. The routine methods for analyzing VOCs include headspace-solid phase microextraction-gas chromatography–mass spectrometry (HS-SPME-GC–MS) and

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headspace gas chromatography–ion mobility spectrometry (HS-GC–IMS). HS-SPME-GC–MS is used for the adsorption and subsequent identification of volatiles in edible oils, offering both qualitative and quantitative results in complex food matrices (Zhou et al., 2024). HS-GC–IMS has advantages such as high sensitivity, fast analysis speed, and simple operation. It is frequently used for discrimination food samples based on VOC profiles (Sun et al., 2023). HS-GC–IMS utilizes the drift time differences of ions in a constant electric field for VOC analysis, making it rather suitable for detecting small-molecule (C2-C10) and trace VOCs. Its results could be a great complement to HS-SPME-GC–MS in the volatile analysis of edible oil (Ma et al., 2023).

Therefore, this study systematically compared the chemical compositions of seed oils from five common Cucurbitaceae species, offering a valuable reference for the comprehensive utilization of Cucurbitaceae resources and the development of high-quality edible oils. The VOCs in these five Cucurbitaceae seed oils were comprehensively analyzed using both HS-GC–IMS and HS-SPME-GC–MS. To our knowledge, this is the first report to systematically research the chemical compositions and volatile flavor profiles of various Cucurbitaceae seed oils.

2. Materials and methods

2.1. Cucurbitaceae seeds and oil extraction

The samples examined in this study consist of the seeds from wax gourd (*Benincasa hispida* (Thunb.) Cogn.), pumpkin (*Cucurbita moschata* Duchesne ex Poir.), watermelon (*Citrullus lanatus* (Thunb.) Matsum. & Nakai), cucumber (*Cucumis sativus* L. var. *sativus*), and bitter gourd (*Momordica charantia* L.). All Cucurbitaceae species were cultivated at the plant base (29°50'–30°13'lat. N; 115°22'–115°49'long. E) of Yunhong Group Co., Ltd. located in Wuxue City, Hubei province, China. These Cucurbitaceae fruits are locally significant crops. All species were harvested in the latter half of 2022, after which the seeds were collected and air-dried at room temperature. The seeds were then stored in dry conditions at ambient temperature, protected from molds, yeasts, and insect infestation.

Except for wax gourd and cucumber seeds, which were challenging to shell, watermelon, pumpkin, and bitter gourd seeds underwent oil extraction after shelling. Given that hot pressing is the predominant technique for extracting oils from fruit and vegetable seeds in commercial production, it also enhances aroma and boosts yield. Consequently, a combined roasting and pressing method was employed using a ZYJ-9018 single-screw oil press (Bestday Co. Ltd., China), which includes stirring-roasting and pressing components, operated under a preset automatic program. Initially, five hundred grams of each seed species were roasted at 130 °C for 13 min, immediately followed by oil extraction using the screw press. Prior to the pressing, the press rod was preheated to 150 °C, and the temperature stabilized around 104 °C during oil release. The extracted oil was separately collected from the outlet, cooled to room temperature, and the centrifugated. The actual oil yield rates were: 19.00 % for wax gourd seeds, 39.30 % for pumpkin seeds, 26.92 % for watermelon seeds, 24.18 % for cucumber seeds, and 21.33 % for bitter gourd seeds. The clarified seed oils were stored in dark glass bottles at 4 °C for further analysis within a month.

2.2. Physicochemical properties of seed oils

The acid values, peroxide value, and iodine value of each seed oil were determined according to GB 5009.229–2016 (National Food Safety Standard of China. Determination of acid value in food), GB/T 5009.227–2016 (National Food Safety Standard of China. Determination of peroxide value in food), and GB/T 5532–2008 (National Standard of China. Animal and vegetable fats and oils. Determination of iodine value), respectively. The oil content in various seeds was determined using the Soxhlet abstracting method in accordance with GB 5009.6–2016 (National Food Safety Standard of China. Determination of fat in food). Total phenolic content was measured using the Folin-C Assay, as previously described by Rao et al. (2021).

2.3. Minerals content analysis

One milliliter of the weighted oil sample was placed in PTFE-coated digestion tubes, followed by the addition of 8.0 mL of concentrated HNO_3 (65 %, *w*/w) to each tube. Subsequently, the sample underwent microwave digestion for 90 min in a graphite acid catcher at 180 °C until the solution turned transparent and reached approximately 1 mL. The solution was then diluted with 2 % HNO_3 up to 10 mL for mineral content detection.

An Agilent 8900 ICP-MS (Agilent Technologies, CA, USA) was used for mineral content determination. High-purity argon gas was used to generate the plasma, and the optimized analysis conditions were as follows: radio frequency power 1550 W, carrier gas 1.0 L/min, auxiliary gas flow rate 1.0 L/min, plasma gas flow rate 15.0 L/min, nebulizer pump 0.1 rps, spray chamber temperature 2 °C, kinetic energy discrimination (KED) mode, with ^{39}K, ^{44}Ca, ^{56}Fe, ^{63}Cu, ^{66}Zn, ^{75}As, ^{78}Se, and ^{111}Cd as quantitative isotopes. A high-purity ICP-MS multi-elements calibration standard solution (ICP-MS Internal Std Mix, Agilent Technologies, CA, USA), containing 10 μg/mL of K, Ca, Fe, Cu, Zn, As, Se, and Cd, was diluted to the appropriate concentrations to establish the standard calibration curve (Ma et al., 2023). Each sample was tested at least in triplicate.

2.4. Determination of fatty acid composition

Fatty acid composition was analyzed following the reported method with modification (Neđeral et al., 2014), involving methyl esterification of fatty acids. Oil sample (60 mg) was weighed into a test tube and dissolved in 4 mL of isooctane. After that, 200 μL of derivatization reagent (2.33 mol/L potassium hydroxide solution in methanol) was added, and the mixture was vortexed for 30 s. Neutralization was achieved by adding 1 g of potassium bisulfate, followed by another 30-s vortexing. The supernatant was filtered through a 0.22 μm membrane filter for analysis.

Fatty acid composition was determined using a 9720 Plus gas chromatograph (Hangzhou Fuli Analytical Instruments Co., Ltd., Zhejiang, China) equipped with a capillary column (RB-FFAP 30 m × 0.32 mm × 0.5 μm, Hangzhou Fuli Analytical Instruments Co., Ltd., Zhejiang, China), a split/splitless injector, and a flame ionization detector. Nitrogen was used as the carrier gas with a flow rate of 1.5 mL/min. The injection volume was 2 μL, with a split ratio of 1:25. The column oven temperature program was as follows: an initial temperature of 120 °C (held for 4 min), ramped to 175 °C at 10 °C/min (held for 6 min), further increased to 210 °C at 5 °C/min (held for 5 min), and finally raised to 230 °C at 4 °C/min (held for 30 min). Both the injector and detector temperatures were maintained at 250 °C. The ignition gases included hydrogen (30 mL/min) and air (300 mL/min). Fatty acids were identified by comparing their retention times with mixed standards of 37-component fatty acid methyl esters (FAME) in isooctane (Yuanye Bio-Technology Co., Ltd., Shanghai, China). Fatty acid content was expressed as a percentage of the total fatty acids.

2.5. Tocopherols analysis

Tocopherol concentrations in the seed oils were determined as follows: 0.5 g of oil sample and 1.0 g of vitamin C were dissolved in 5 mL of *n*-hexane. Then, 5 mL of methanol aqueous solution (90:10, *v*/v) was added to extract the tocopherols, and the mixture was vortexed for 2 min. After centrifugation, the methanol aqueous phase was collected, and the extraction process was repeated twice. The combined methanol aqueous phases were then diluted to 10.0 mL with 90 % methanol aqueous solution. Prior to HPLC analysis, the samples were filtered through a 0.22 μm membrane filter. HPLC conditions were based on

reported methods with minor modifications (Hu et al., 2023). External standards of α-, β-, γ-, and δ-tocopherols (Aladdin Biochemical Technology Co., Ltd., Shanghai, China) were used to calculate the individual tocopherol amounts in oil samples. The samples were eluted with 98 % (*v*/v) methanol aqueous solution at a flow rate of 1.0 mL/min using an Alltech 1500 HPLC system (SSI, PA, US) equipped with a DAD detector and a CSChromPlus chromatography workstation. The sample injection volume was 10 μL, and the detection wavelength was set to 300 nm. Separation was achieved using a Luna C18 Phenomenex column (250 mm × 4.6 mm × 5 μm). Tocopherol content was expressed in parts per million relatives to the oil. Each sample was tested in triplicate.

2.6. Squalene content

The determination of the squalene content was carried out using the method of Zhao et al. (2019) with minor modifications. A mixture of 0.50 g of each seed oil and 4 mL of 2 M KOH ethanol solution was sonicated at 75 °C for 40 min. Subsequently, 4 mL of water and 3 mL of *n*-hexane were added, and the mixture was vortexed for 5 min. After centrifugation, the *n*-hexane layer was collected. The extraction process was repeated twice more, each time with 3 mL of *n*-hexane. The combined *n*-hexane phases were then dried by nitrogen stripping. The dry unsaponifiable matter was dissolved in 5 mL of *n*-hexane and filtered through a 0.22 μm membrane filter before analysis. Each sample was explored in triplicate.

Squalene content was determined by EXPEC 5231 GC–MS (EXPEC Technology, Hangzhou, China) equipped with a DB-5MS column (30 m × 250 μm × 0.25 μm, Agilent Technologies, USA). The injection volume was 2 μL, with helium as carrier gas at a flow rate of 1 mL /min, and an injection temperature of 280 °C. The temperature was initially kept at 200 °C for 1 min, increased to 300 °C at 20 °C/min, and held at 300 °C for 5 min. The MS parameters included an electronic ionization voltage of 70 eV, an ion source temperature of 250 °C, and SIM mode targeting ions 81 *m/z*, 95 *m/z*, and 137 *m/z*, with a qualifier ion 69 *m/z*. Calibration curves were generated using external squalene standards (Shanghai Yuanye Bio-Technology Co., Ltd., Shanghai, China) to calculate squalene content in the oil samples.

2.7. HS-GC–IMS analysis

HS-GC–IMS analysis was conducted to differentiate the five seed oils. VOCs in the samples were analyzed using an HS-GC–IMS (FlavourSpec®, Gesellschaft für analytische Sensorsysteme mbH, Dortmund, Germany) equipped with a PAL HS-xt autosampler (CTC Analytics AG, Zwingen, Switzerland), a 490 micro gas chromatograph (Agilent Technologies, CA, USA), and a drift time IMS cell. Briefly, each sample (1.0 g) was placed in a 20 mL headspace vial and incubated at 80 °C for 15 min. Subsequently, 500 μL of headspace was automatically loaded into the injector using a heated syringe at 85 °C. The GC was equipped with an FS-SE-54-CB-1 capillary column (15 m × 0.53 mm × 1.0 μm) at 45 °C. Nitrogen (99.99 % purity) was used as the carrier gas with a linear pressure program as follows: 2 mL/min for 2 min, linearly increased to 10 mL/min for 2–10 min, linearly increase to 100 mL/min over 10–20 min, and ramp up to 150 mL/min for 20–30 min. The pre-separated compounds were ionized and further transferred to the 9.8 cm drift tube, which operated at a constant voltage (5 kV) at 45 °C under 150 mL/min flowing nitrogen. C4–C9 *n*-ketones (Sinopharm Chemical Reagent, Beijing, China) were used as external references to calculate the retention index (RI) of VOCs through the automated mass spectral deconvolution and identification system. VOCs were identified by comparing their retention times, ion drift times, and RI values of the standard signals in the GC–IMS library.

Data analyses were conducted using the LAV software version 2.2.1 (Gesellschaft für analytische Sensorsysteme mbH, Dortmund, Germany). The Gallery Plot plugin was used to export the fingerprint spectrum and analyze the VOC differences in samples. The fingerprint information was obtained from the peak volumes for all the VOCs resolved in the topographic plots which generated by the Reporter plugin. The intensity (a.u.) was obtained through the LAV plugin and expressed as the integral area.

2.8. HS-SPME-GC–MS analysis

HS-SPME-GC–MS analysis was performed following the published method with minor modifications (Zhou et al., 2024). HS-SPME was conducted using an MPS2 programmable robotic multipurpose sampler (Gerstel, Mülheim an der Ruhr, Germany) equipped with a 50/30 μm DVB/CAR/PDM fiber (Supelco, Bellefonte, PA, United States). Briefly, 3.0 g of sample was placed in a 20 mL SPME vials, and 30 μL of ethanol containing 3 μg of 2-methyl-3-heptanone (Sigma-Aldrich, St. Louis, MO, USA) as the internal standard was added, and the vial was sealed. Prior to extraction, the SPME fiber was preconditioned by heating at the injection port (250 °C) for 40 min. Samples were then preequilibrated at 60 °C for 20 min and extracted by the SPME fiber for 30 min at the same temperature under stirring at 250 rpm. Upon completion, the fiber was immediately inserted into the injection port of the GC–MS for 8 min.

GC–MS analysis was conducted using an EXPEC 5231 gas chromatograph–mass spectrometer (EXPEC Technology, Hangzhou, China). A DB-5MS column (30 m × 250 μm × 0.25 μm, Agilent Technologies, USA) was used, and high purity helium (99.99 %) was utilized as the carrier gas at a flow rate of 1.0 mL/min. Heating procedure was as follows: the initial temperature was 40 °C for 2 min, then increased to 240 °C at 5 °C/min and held at 240 °C for 3 min, and a splitless model was set. The mass-selective detector was operated in electron-impact ionization (EI) mode with a mass scan range from *m/z* 30 to 500 at 70 eV. The temperature of ion source was set at 250 °C.

VOCs were identified by matching their MS spectra with data from the NIST 14 library and comparing the calculated RI values with reported RI values. Compounds derived from the column, known contaminants, and compounds with both matching and reverse matching degrees lower than 800 were excluded from the analysis. C5–C30 *n*-alkanes (Sigma–Aldrich Co., Ltd., Shanghai, China) were applied as external references for RI calculation. The relative concentration of each VOC was calculated by the ratio of the peak area to the internal standard. Each sample was analyzed in triplicate.

2.9. Statistical analysis

Results are expressed as mean ± standard deviation ($n = 3$). SPSS 27.0 software was used for one-way analysis of significant differences ($p < 0.05$) among samples. Principal component analysis (PCA) was conducted using MetaboAnalyst 6.0 (https://www.metaboanalyst.ca). To ensure the optimum comparability in feature magnitudes, sum normalization was employed for the HS-GC–IMS model, whereas median normalization and mean centering were selected for the HS-SPME-GC–MS model.

3. Results and discussion

3.1. Physicochemical properties

The physicochemical properties of five seed oils are summarized in Table 1. Significant variations in oil content were observed among the different seed types. Pumpkin seeds exhibited the highest oil content at 44.91 ± 4.50 %, while wax gourd seeds exhibited the lowest concentration at 24.35 ± 2.08 %. The acid value, which reflects the free fatty acid content in oils, varied considerably, with WGSO displaying the highest value (2.02 ± 0.14 mg KOH/g oil) and WSO the lowest (0.31 ± 0.06 mg KOH/g oil). The remaining oils had similar acid values, ranging from 1.21 to 1.34 mg KOH/g oil. The peroxide value indicates the degree of oil oxidation. All the seed oils in our study exhibited low peroxide values, indicating their freshness and quality. The iodine value, which

Table 1
Physicochemical properties of five *Cucurbitaceae* seed oils.

Property	WGSO	PSO	WSO	CSO	BGSO
Oil content (% w/w)	24.35 ± 2.08^{c}	44.91 ± 4.50^{a}	32.16 ± 1.27^{b}	30.72 ± 2.54^{b}	34.93 ± 1.40^{b}
Acid value (mg KOH/g oil)	2.02 ± 0.14^{a}	1.21 ± 0.16^{b}	0.31 ± 0.06^{c}	1.32 ± 0.13^{b}	1.34 ± 0.14^{b}
Peroxide value (meq O_2/100 g oil)	0.026 ± 0.001^{d}	0.039 ± 0.001^{b}	0.078 ± 0.001^{a}	0.021 ± 0.001^{e}	0.037 ± 0.001^{c}
Iodine value (g iodine/100 g oil)	144.47 ± 2.48^{a}	114.90 ± 1.70^{c}	63.65 ± 0.94^{e}	87.38 ± 0.90^{d}	141.25 ± 1.49^{b}
Total Phenolics (mg gallic/kg oil)	229.12 ± 1.55^{c}	185.53 ± 1.24^{d}	276.48 ± 4.06^{b}	179.90 ± 1.56^{e}	321.85 ± 2.14^{a}

^{a,b,c,d,e} Values in the same row with different letters are significant difference at $p < 0.05$, results are expressed as mean ± standard deviation ($n = 3$).

reflects oil unsaturation, showed that WGSO (144.47 ± 2.48 g iodine/100 g oil) and BGSO (141.25 ± 1.49 g iodine/100 g oil) had significantly higher iodine values, indicating a higher level of unsaturation compared to other oils. Additionally, all the oils exhibited considerable phenolic content, with BGSO exhibiting the highest phenolic content at 321.85 ± 2.14 mg gallic/kg oil. These physicochemical properties are consistent with literature findings for WSO (Angelova-Romova et al., 2019), PSO (Nawirska-Olszańska et al., 2013), WGSO (Yao et al., 2019), CSO (Murthy et al., 2022), and BGSO (Lee et al., 2015).

3.2. Mineral content

Minerals are crucial in human health, which serve as important food quality indicators (Juranovic et al., 2003). In this study, six essential minerals (K, Ca, Fe, Cu, Zn, and Se) and two potentially harmful elements (As and Cd) were determined using ICP-MS (Table 2). K was the most abundant mineral in all seed oils, whereas Ca levels were lower. Among the trace elements, Fe had the highest content (0.05–5.71 mg/kg), followed by Zn (0.13–0.69 mg/kg), with lower levels of Cu and Se. As and Cd were present in trace amounts. WGSO and BGSO had the highest mineral content, particularly in four trace elements essential for human health. For example, WGSO contained 5.71 ± 0.54 mg/kg Fe and 0.497 ± 0.043 mg/kg Se. In contrast, WSO had the lowest mineral content, except for Zn (0.61 ± 0.04 mg/kg). While PSO did not have the highest overall mineral content, it had the highest K level (28.98 ± 0.95 mg/kg). The mineral contents in PSO, including Ca, K, Cd, Cu, Fe, and Zn were consistent with the finding of Juranovic et al. (2003). In addition, the minerals in WSO and PSO fell within the ranges reported for watermelon and pumpkin seeds (El-Adawy & Taha, 2001; Jafari et al., 2012).

Mineral content in fruits and vegetables is influenced by various factors such as soil composition, fertilizers, climate, growth cycle, and production processes (Joebstl et al., 2010; Mi et al., 2022). Soil composition directly affects the mineral composition and content of plants. Additionally, different Cucurbitaceae species vary in their ability to accumulate minerals (Murthy et al., 2022). Although our results may not represent all Cucurbitaceae fruits and their products in the market, the fact that our study vegetables were cultivated at the same location provides valuable insights into the mineral profiles of different Cucurbitaceae seed oils. Moreover, the significant differences in mineral content among these seed oils offer a new approach for the rapid discrimination of various seed oils (Joebstl et al., 2010).

3.3. Fatty acid profile

Although extensive research has been conducted on fatty acid compositions of various fruits and vegetables seed oils (Yao et al., 2019), this study represents the first simultaneous exploration of the lipid profiles of seed oils from five common Cucurbitaceae species. Table 3 presents the fatty acid composition of five Cucurbitaceae seed oils. Cucurbitaceae seed oils are generally rich in unsaturated fatty acids, with the total unsaturated fatty acid (UFA) content ranging from 70.12 % in BGSO to 84.07 % in WSO.

The fatty acid compositions of WSO, PSO, WGSO, and CSO were closely aligned, with linoleic acid (C18:2), all dominated by oleic acid (C18:1), palmitic acid (C16:0), and stearic acid (C18:0). These results align with previous publications on these seed oils (Lee et al., 2015; Stevenson et al., 2007; Yao et al., 2019). Linoleic acid was the dominant fatty acid in the four samples, accounting for over 65 % of the total fatty acid content, except in PSO where it was lower (47.49 %). WSO and CSO represented the highest linoleic acid content, with 73.68 % and 72.11 %, respectively, which is consistent with previous studies (Murthy et al., 2022; Yao et al., 2019). Linoleic acid, an essential fatty acid vital for skin and cell membrane integrity, immune system function, and eicosanoid synthesis, cannot be synthesized by the human body and must be obtained through diet. Therefore, these four seed oils could serve as excellent dietary sources of linoleic acid. Among the monounsaturated acids, oleic acid occurs in the greatest amount in PSO (31.45 %), which is within the reported range for twelve varieties of PSO (Nawirska-Olszańska et al., 2013). Whereas WSO, WGSO, and CSO contained approximately 10 % of oleic acid. Additionally, the low linolenic acid content (C18:3 < 1 %) in these four seed oils can contribute to their high oxidative stability and prolonged shelf life (Stevenson et al., 2007).

α-Eleostearic acid (EA, C18:3 9c11t13t), a long-chain polyunsaturated fatty acid (ω-5) with conjugated double bonds, has been reported as the main component of BGSO (more than 50 %) (Saha et al., 2012). In this study, EA accounted for 55.38 % of BGSO, while catalpic acid (C18:3 9t11t13c) reached 5.03 %, concurring with previous research on BGSO (Yoshime et al., 2016; Yoshime et al., 2019). Notably, EA was absent in the other four oil samples. Additionally, BGSO had the highest saturated fatty acid content (27.50 %) among the five seed oils, with stearic acid being the most abundant (26.03 %). This high saturated fatty acid content leads to BGSO solidifying at room temperature, in contrast to the liquid state of the other four seed oils. Furthermore, while oleic acid and linoleic acid dominant the other four seed oils, they only accounted for 5.07 % and 4.05 % respectively in BGSO.

3.4. Tocopherols and squalene content

The β- and γ-tocopherol isomers, which differ by a single methyl group on the benzene ring (in para and ortho positions, respectively), showed overlapping retention times and signal peaks under our HPLC conditions. Therefore, we provide the combined content of β- and

Table 2
Mineral compositions (mg/kg) in *Cucurbitaceae* seed oils.

Sample	Potassium (K)	Calcium (Ca)	Iron (Fe)	Copper (Cu)	Zinc (Zn)	Selenium (Se)	Arsenic (As)	Cadmium (Cd)
WGSO	14.68 ± 1.12^{b}	2.45 ± 0.27^{a}	5.71 ± 0.54^{a}	0.062 ± 0.005^{b}	0.52 ± 0.04^{c}	0.497 ± 0.043^{a}	0.0078 ± 0.0005^{a}	0.0004 ± 0.0001^{a}
PSO	28.98 ± 0.95^{a}	0.89 ± 0.04^{c}	0.38 ± 0.10^{d}	0.035 ± 0.001^{c}	0.34 ± 0.04^{d}	0.021 ± 0.003^{b}	0.0004 ± 0.0001^{c}	–
WSO	6.75 ± 0.34^{d}	0.98 ± 0.04^{c}	0.05 ± 0.02^{d}	–	0.61 ± 0.04^{b}	0.008 ± 0.001^{b}	0.0002 ± 0.0001^{c}	–
CSO	10.19 ± 0.44^{c}	1.45 ± 0.10^{b}	1.49 ± 0.13^{c}	0.011 ± 0.001^{d}	0.13 ± 0.01^{e}	0.013 ± 0.001^{b}	0.0007 ± 0.0002^{c}	–
BGSO	15.60 ± 0.29^{b}	1.06 ± 0.05^{c}	2.55 ± 0.13^{b}	0.069 ± 0.002^{a}	0.69 ± 0.03^{a}	0.013 ± 0.001^{b}	0.0062 ± 0.0006^{b}	0.0005 ± 0.0001^{a}

^{a,b,c,d,e} Values in the same column with different letters are significant difference at $p < 0.05$, results are expressed as mean ± standard deviation ($n = 3$).

Table 3
Fatty acid composition (% of total, mean ± SD) of five *Cucurbitaceae* seed oils.

Fatty acids	WGSO	PSO	WSO	CSO	BGSO
C14:0[#]	0.03 ± 0.00[b]	0.07 ± 0.00[a]	0.02 ± 0.00[c]	0.03 ± 0.00[b]	–
C16:0	11.19 ± 0.07[b]	11.31 ± 0.04[a]	8.46 ± 0.05[d]	10.65 ± 0.03[c]	1.04 ± 0.00[e]
C16:1	0.05 ± 0.01[c]	0.09 ± 0.00[a]	0.05 ± 0.01[c]	0.07 ± 0.00[b]	–
C17:0	0.05 ± 0.00[b]	0.06 ± 0.00[a]	0.04 ± 0.00[e]	0.04 ± 0.00[d]	0.05 ± 0.00[c]
C17:1	–	0.03 ± 0.00	–	–	–
C18:0	7.58 ± 0.06[b]	6.86 ± 0.00[c]	5.83 ± 0.00[d]	4.97 ± 0.01[e]	26.03 ± 0.06[a]
C18:1	10.73 ± 0.02[b]	31.45 ± 0.21[a]	9.60 ± 0.00[c]	8.59 ± 0.01[d]	5.07 ± 0.08[e]
C18:2	67.50 ± 0.27[c]	47.49 ± 0.04[d]	73.68 ± 0.11[a]	72.11 ± 0.07[b]	4.05 ± 0.01[e]
α-C18:3	0.25 ± 0.01[b]	0.16 ± 0.00[c]	0.09 ± 0.00[d]	0.35 ± 0.00[a]	–
γ-C18:3	0.24 ± 0.01[c]	0.33 ± 0.00[a]	0.16 ± 0.00[d]	0.13 ± 0.00[e]	0.28 ± 0.01[b]
C18:3 9c11t13t	–	–	–	–	55.38 ± 0.12
C18:3 9t11t13c	–	–	–	–	5.03 ± 0.12
C20:0	0.07 ± 0.00[c]	0.09 ± 0.00[b]	0.07 ± 0.01[c]	0.06 ± 0.00[d]	0.24 ± 0.00[a]
C20:1	–	–	–	–	0.05 ± 0.01
C21:0	–	–	–	–	0.03 ± 0.01
C22:0	–	–	–	–	0.06 ± 0.01
C20:3	0.05 ± 0.01[c]	0.08 ± 0.00[b]	0.04 ± 0.01[d]	0.02 ± 0.00[e]	0.12 ± 0.01[a]
C20:4	0.15 ± 0.00[b]	0.06 ± 0.00[c]	–	0.72 ± 0.00[a]	
C23:0	0.20 ± 0.01[a]	0.12 ± 0.01[b]	0.02 ± 0.01[e]	0.10 ± 0.00[c]	0.03 ± 0.01[d]
C22:2	0.03 ± 0.01[d]	0.06 ± 0.01[b]	0.04 ± 0.00[c]	0.08 ± 0.00[a]	–
C24:0	0.06 ± 0.01[a]	0.06 ± 0.01[a]	0.04 ± 0.00[b]	0.03 ± 0.00[b]	0.03 ± 0.00[b]
C20:5	0.07 ± 0.02[b]	0.31 ± 0.02[a]	0.07 ± 0.00[b]	0.06 ± 0.01[b]	–
C24:1	0.09 ± 0.01[ab]	0.20 ± 0.00[a]	0.11 ± 0.04[ab]	0.06 ± 0.00[b]	0.07 ± 0.00[b]
C22:6	0.62 ± 0.01[a]	0.34 ± 0.01[c]	0.24 ± 0.00[d]	0.44 ± 0.00[b]	0.06 ± 0.01[e]
Saturated	19.18 ± 0.17[b]	18.56 ± 0.07[c]	14.47 ± 0.08[e]	15.88 ± 0.04[d]	27.50 ± 0.10[a]
Unsaturated	79.78 ± 0.36[d]	80.59 ± 0.28[c]	84.07 ± 0.28[a]	82.63 ± 0.09[b]	70.12 ± 0.35[e]
Monounsaturated	10.87 ± 0.03[b]	31.76 ± 0.21[a]	9.76 ± 0.16[c]	8.72 ± 0.01[d]	5.19 ± 0.09[e]
Polyunsaturated	68.91 ± 0.33[c]	48.83 ± 0.07[e]	74.31 ± 0.12[a]	73.91 ± 0.08[b]	64.93 ± 0.26[d]

[#] Fatty acid abbreviations are as follows: C14:0, Myristic Acid; C16:0, Palmitic Acid; C16:1, Palmitoleic Acid; C17:0, Heptadecanoic acid; C17:1, cis-10-Heptadecenoic Acid; C18:0, Stearic Acid; C18:1, Oleic Acid; C18:2, Linoleic Acid; α-C18:3, α-Linolenic Acid; γ-C18:3, γ-Linolenic Acid; C18:3 9c11t13t, α-eleostearic acid; C18:3 9t11t13c, catalpic acid; C20:0, Arachidic Acid; C20:1, cis-11-Eicosenoic Acid; C21:0, Heneicosanoic Acid; C22:0, Behenic Acid; C20:3, cis-8,11,14-Eicosatrienoic Acid; C20:4, Arachidonic Acid; C23:0, Tricosanoic Acid; C22:2, cis-13,16-Docosadienoic Acid; C24:0, Lignoceric Acid; C20:5, Eicosapentaenoic Acid; C24:1, Nervonic Acid; C22:6, Docosahexaenoic acid.
[a,b,c,d,e] Values in the same row with different letters are significant difference at $p < 0.05$, results are expressed as mean ± standard deviation (n = 3).

γ-tocopherol based on the overlapping signals, in line with previous studies (Ryan et al., 2007; Stevenson et al., 2007). The HPLC spectra of five seed oils and standards are presented in Fig. S1. Significant variations in tocopherol composition and total content were observed among the five seed oils (Table 4). WSO exhibited the highest total tocopherol content (1476.39 mg/kg), primarily consisting of δ-tocopherol (1369.93 mg/kg). WGSO followed closely with a total tocopherol content of 1111.63 mg/kg, in agreement with previous findings that γ-tocopherol is the dominant form (Yao et al., 2019).

The remaining three seed oils had significantly lower total tocopherol content, with PSO containing 195.37 mg/kg. This value aligns with the total tocopherol content in PSO reported by Yao et al. (2019), though this study identified β-tocopherol as the primary tocopherol species. In the present study, δ-tocopherol was detected as the dominant form in PSO, consistent with previous reports that 11 of 12 PSO varieties mainly contained δ-tocopherol, with only one cultivar (Big Max) having a higher content of β-tocopherol (Stevenson et al., 2007). Conversely, Nawirska-Olszańska et al. (2013) reported that γ-tocopherol was the main tocopherol in seed oils of 12 pumpkin cultivars. This highlights the significant variation in tocopherol species across different pumpkin cultivars. BGSO displayed lower total tocopherol content (92.04 mg/kg), with δ-tocopherol as the primary species consistent with the previous findings (Yoshime et al., 2019). Finally, CSO exhibited the lowest tocopherol content (18.84 mg/kg) and was the only seed oil without α-tocopherol detected. The tocopherol species composition in CSO was consistent with the report by Matthaus et al. (2003), but the total content was lower.

Squalene is a polyunsaturated hydrocarbon widely found in animals and plants. Researchers are interested in squalene for its biological activities and its applications in food and cosmetics. Squalene serves as a precursor for synthetic steroid substances, such as phytosterols. It is more abundant in shark liver oil and olive oil than in most other vegetable oils (Yao et al., 2019). PSO had a significantly higher squalene content than the other four seed oils, reaching 1511.74 mg/kg (Table 4), a level comparable to that found in olive oil (Beltrán et al., 2015). This result is similar to the squalene content in PSO reported by Qi et al. (2012) (920 to 1290 mg/kg) but is lower than the 2732 mg/kg reported by Yao et al. (2019), suggesting potential variations due to differences in pumpkin varieties and growth conditions. Overall, PSO stands out as a promising source of squalene for various industrial applications. WGSO, WSO, and CSO had similar squalene contents, ranging from 554.84 to 682.77 mg/kg, which are higher than the values reported for some seeds, grains, and legumes (Ryan et al., 2007). Additionally, the squalene content (682.77 mg/kg) in WSO surpassed the reported values (113.7 mg/kg) (Yao et al., 2019). By contrast, BGSO had the lowest squalene content, only 48.80 mg/kg.

3.5. VOC fingerprints of five seed oils by HS-GC–IMS

HS-GC–IMS was applied to study the volatile profiles of Cucurbitaceae seed oils for the first time. A total of 118 VOCs were identified in five seed oils, comprising 32 alcohols, 17 aldehydes, 29 esters, 17 ketones, 3 ethers, 9 acids, and 11 other compounds (Table 5). These results corresponded to the previous publications that most of the volatiles in roasted Cucurbitaceae seeds were lipid oxidation and Strecker degradation products, such as aliphatic aldehydes, ketones, and alcohols (Bowman & Barringer, 2012; Siegmund & Murkovic, 2004). Notably, eight substances were detected in both monomer and dimer forms due to their high proton affinity or concentration, which can lead to multiple signals during a single analysis (Ma et al., 2023).

The Gallery Plot plugin generated a comparative analysis of the fingerprint spectra, highlighting differences in VOC composition across the seed oils (Fig. 1). The horizontal axis represents the five seed oils, and the vertical axis denotes the VOCs. Each square symbolizes a VOC and its normalized intensity in a specific seed oil, with a redder area indicating a stronger signal intensity. Fig. 1A illustrates thirteen common VOCs across the five seed oils, including 2-methylpropanal (M), tetrahydrofuran, 1-propanethiol, and methyl butyrate with significant peak volumes (Table 5). 2-methylpropanal, associated to the pungent and malt odors in edible oil, is generated by Strecker degradation of

Table 4
Content (mg/kg) analysis of squalene and tocopherols in five seed oils.

	WGSO	PSO	WSO	CSO	BGSO
Squalene	597.87 ± 78.75^{bc}	1511.74 ± 87.88^{a}	682.77 ± 27.15^{b}	554.84 ± 17.59^{c}	48.80 ± 2.90^{d}
Tocopherol					
α- tocopherol	380.21 ± 57.91^{a}	17.12 ± 4.26^{b}	9.42 ± 1.63^{b}	ND	4.84 ± 0.42^{b}
β + γ- tocopherol$^{\#}$	459.22 ± 12.75^{a}	9.92 ± 0.95^{c}	97.04 ± 13.27^{b}	7.41 ± 5.14^{c}	16.69 ± 10.23^{c}
δ- tocopherol	272.20 ± 35.66^{b}	168.33 ± 8.15^{c}	1369.93 ± 27.91^{a}	11.43 ± 4.78^{e}	70.51 ± 9.18^{d}
Total	1111.63^{b}	195.37^{c}	1476.39^{a}	18.84^{e}	92.04^{d}

ND, not detected;
^{a,b,c,d,e} Values in the same row with different letters are significant difference at $p < 0.05$, results are expressed as mean ± standard deviation (n = 3);
$^{\#}$ signals of β-, and γ-tocopherol isomers are overlapped in present HPLC conditions.

valine during roasting of the seeds (Zhang et al., 2021). Specifically, the monomer form of 2-methylpropanal is the most abundant volatile compound across the five samples. This result is consistent with the previous studies showing that 2-methylpropanal is one of the Strecker aldehydes with highest concentration in roasted pumpkin seeds (Bowman et al., 2012). Fig. 1B highlights twenty-six VOCs with significantly higher content in WGSO, PSO, CSO, and WSO. Among them, 3-methylbutanal exhibited significantly higher peak volumes, particularly in WGSO and PSO. 2-Methylbutanal and 3-methylbutanal, formed form Strecker degradation of leucine and isoleucine, are the important volatile compounds contributing to the unique roasted aroma of pumpkin seeds (Bowman et al., 2012). Their concentration in roasted pumpkin seeds can increase significantly when the roasting temperature rises above 100 °C (Siegmund et al., 2004). Additionally, 2-butanol (M) and trans-2-Hexen-1-ol showed higher peak volumes in CSO and PSO, respectively. 2,3-Butanediol with fruity aroma was previously identified in roasted WSO (Ok & Yilmaz, 2019), and isoamyl alcohol was also detected at low concentration on volatile oil of bitter gourd (Moronkola et al., 2009). Moreover, acetoin has been identified as the key odor active compound in wax gourd fruit (Sharma et al., 2010).

Fig. 1C shows thirteen VOCs abundant in WGSO and BGSO, including methyl acetate, 2-methylpropanal (D), and isopropyl alcohol, which had higher intensities than other VOCs. This suggests WGSO could be the most similar seed oil to BGSO compared to others. Methyl acetate, previously detected in sunflower seed oil VOCs, can contribute to a fruity aroma. It is likely produced by the decomposition of hydroperoxides formed during oil oxidation (Liu et al., 2023). 2-Methylpropanal, a Strecker aldehyde commonly detected in PSO, is formed by Strecker degradation of amino acids during the Maillard reaction and is important to roasted aroma (Bowman et al., 2012; Gaca et al., 2021). Isopropyl alcohol has also been detected in the volatile oil of bitter gourd (Moronkola et al., 2009). Fig. 1D shows eight VOCs with higher content in WGSO, including furfural, which was previously detected in roasted rapeseed oil (Zhang et al., 2021), flaxseed oil (Sun et al., 2023), and WSO (Ok et al., 2019). Furans as a major class of volatiles formed by lipid peroxidation, carbohydrate degradation, and Maillard reaction, giving sweet, malty, and caramel aromas to food (Zhang et al., 2021). Beta-ocimene was previously reported abundant in black cumin oil, which was one the most significant volatiles that were responsible for the differences apart from other seed oils (Gaca et al., 2021). Additionally, four VOCs were abundant in CSO, including cis-4-heptenal, 3-heptanol, 3-methyl-2-butanol, and ethyl formate. It is reported that cis-4-heptenal can contribute to a fishy smell in seed oil, but the specific odor feature of this compound remains under dispute (Zhang et al., 2021). Moreover, Fig. 1E highlights fifty-three VOCs unique to BGSO, primarily comprising sixteen alcohols, twelve esters, eight aldehydes, seven ketones, and four acids. These results were in agreement with previous studies, which found aliphatic alcohols to constitute that major class of compounds identified from the volatile oil of bitter guard. Specifically, the detected VOCs in BGSO such as trans-2-hexenal, cis-2-penten-1-ol, 3-octanol, nerol, octanal, 2,6-dimethylpyrazine, trans-3-hexen-1-ol, and 2-hexanol, were also identified in the volatile oil of bitter guard using GC–MS previously (Moronkola et al., 2009).

3.6. VOC profiles in five seed oils by HS-SPME-GC–MS

HS-SPME-GC–MS was used to comprehensively analyze the VOC profiles of five seed oils. A total of sixty-seven VOCs were identified, including eighteen alcohols, seventeen aldehydes, five esters, six ketones, three acids, four pyrazines, one phenol, and thirteen other compounds (Table 6). Compared to HS-GC–IMS, HS-SPME-GC–MS detected fewer VOCs. This difference may be attributed to several factors. Similar to HS-GC–IMS, most of the analytes were products of lipid oxidation, carbohydrates degradation, Strecker degradation, and Maillard reactions, such as alcohols, aldehydes, ketones, and pyrazines (Gaca et al., 2021; Zhang et al., 2021). These compounds are prevalent C3-C10 molecules with high volatile features, within the detection range of HS-GC–IMS. Moreover, most of these VOCs are present at low concentrations in the lipid headspace, making them easier to detect by HS-GC–IMS due to its sensitivity, even at trace levels. While HS-SPME-GC–MS stands as a widely used method for detecting volatile components in edible oils, it suffers from limitations such as susceptibility to the matrix effect of oil during extraction, selectivity issues, and challenges in extracting trace-level compounds (Suzuki et al., 2020). However, HS-SPME-GC–MS has the advantage of accurately identifying VOCs and providing quantitative results by comparison with standards.

In terms of VOC abundance and categories, HS-SPME-GC–MS exhibited similar results to HS-GC–IMS. The total ion chromatogram is given in Fig. S2, with BGSO containing the most abundant VOCs. Alcohols including straight-chain and branched alcohols are the third largest group of volatiles in vegetables besides aldehydes and ketones (Zhang et al., 2021). In this assay, alcohols were the prevalent VOCs in the headspace of seed oils. 1-Pentanol primarily originating from lipid oxidation in edible oils, was found at the highest concentration in BGSO, reaching 287.29 ± 9.98 mg/kg (Table 6). Additionally, other alcohols detected in BGSO, such as isoamyl alcohol, 1-hexanol, benzyl alcohol, 2-phenylethanol, and 2,4-nonadien-1-ol were also identified in the essential oils of bitter gourd fruits and leaves (Ferreira Almeida et al., 2024; Moronkola et al., 2009). In contrast, WGSO had the most abundant content of alcohols among the remaining samples. Except for benzyl alcohol and 2-phenylethanol, which are commonly found in Cucurbitaceae seed oils (Siegmund & Murkovic, 2004), WGSO contained 15.99 ± 1.87 mg/kg of 2,3-butanediol, a compound previously reported in high levels in roasted argan oil (Gaca et al., 2021). In contrast, only three alcohols were detected in CSO, including benzyl alcohol, 2-phenylethanol, and 1-hexanol. Where 1-hexanol (31.27 ± 1.60 mg/kg) exhibited a significantly higher content in CSO than other samples. 1-Hexanol is typically considered a characteristic C6 volatile alcohol in cucumber fruits (Shan et al., 2020). PSO and WSO shared similar alcoholic compounds, with 1-hexanol, 1-octen-3-ol, and 2-phenylethanol as their common VOCs.

Aldehydes are common volatiles in vegetable oils, formed by fatty acid oxidation or Strecker degradation (Zhang et al., 2021). HS-SPME-GC–MS detected a diverse range of alcohols in CSO, among which benzaldehyde was the most abundant at 6.04 ± 1.05 mg/kg. This result corresponded to previous reports that benzaldehyde was one of the aroma-active compounds in five different cucumber fruits (Mi et al.,

Table 5
The VOC compositions and integral parameters of five seed oils based on HS-GC–IMS.

IMS Code	VOCs	CAS	Formular	Retention time [*sec*]	Retention index*	Drift time [RIP relative]	Peak volume (a.u.)				
							WGSO	PSO	WSO	CSO	BGSO
Alcohols (31)											
1	Benzyl alcohol	100–51-6	C7H8O	687.056	1028.9	1.1623	316.33 ± 12.50^{a}	341.33 ± 7.37^{a}	219.00 ± 50.48^{b}	170.67 ± 15.18^{c}	71.67 ± 5.51^{d}
2	4-Hexen-1-ol	6126-50-7	C6H12O	370.769	881.5	1.4843	127.00 ± 8.19^{c}	160.00 ± 2.65^{b}	80.67 ± 20.82^{d}	137.33 ± 5.69^{c}	208.33 ± 8.02^{a}
4	3-Heptanol	589–82-2	C7H16O	368.878	880.3	1.6449	72.33 ± 24.85^{c}	70.00 ± 10.82^{c}	47.00 ± 7.55^{c}	401.67 ± 19.43^{a}	177.67 ± 15.89^{b}
13	2,3-Butanediol	513–85-9	C4H10O2	237.221	798.4	1.3665	157.67 ± 62.98^{a}	148.33 ± 9.29^{a}	117.00 ± 3.00^{ab}	125.00 ± 4.36^{ab}	84.33 ± 6.11^{b}
16	2-Hexanol	626–93-7	C6H14O	619.329	992.7	1.5727	41.67 ± 2.89^{c}	63.67 ± 0.58^{b}	27.67 ± 3.79^{d}	31.67 ± 2.89^{d}	199.33 ± 6.66^{a}
17	1-Heptanol	111–70-6	C7H16O	546.384	960.8	1.3838	146.67 ± 6.66^{a}	112.67 ± 4.04^{b}	72.33 ± 9.45^{c}	71.33 ± 8.08^{c}	99.00 ± 11.53^{b}
20	trans-2-Hexen-1-ol	928–95-0	C6H12O	389.824	892.6	1.1645	296.67 ± 23.29^{b}	421.33 ± 6.03^{a}	232.00 ± 94.94^{bc}	174.00 ± 13.75^{c}	155.33 ± 57.06^{c}
25	4-Methyl-2-pentanol	108–11-2	C6H14O	182.749	752.1	1.2842	164.00 ± 21.93^{a}	98.33 ± 2.52^{b}	87.33 ± 4.16^{b}	98.33 ± 1.53^{b}	79.33 ± 9.45^{b}
26	Isoamyl alcohol	123–51-3	C5H12O	173.342	743.5	1.2458	191.33 ± 20.03^{a}	107.33 ± 6.03^{c}	137.33 ± 2.52^{b}	177.67 ± 4.16^{a}	71.00 ± 11.53^{d}
38	Isopropyl alcohol	67–63-0	C3H8O	52.393	594.6	1.2515	490.67 ± 28.99^{b}	373.33 ± 8.08^{c}	141.33 ± 2.31^{e}	245.33 ± 6.03^{d}	550.33 ± 9.24^{a}
96	2-Butanol (M)	78–92-2	C4H10O	48.658	589.0	1.1458	272.33 ± 8.96^{d}	335.00 ± 3.46^{c}	444.33 ± 14.36^{b}	642.67 ± 2.52^{a}	256.33 ± 32.93^{d}
42	2-Butanol (D)	78–92-2	C4H10O	79.423	635.4	1.3226	432.00 ± 33.15^{a}	209.00 ± 9.64^{b}	75.00 ± 1.00^{d}	135.33 ± 7.51^{c}	211.67 ± 11.55^{b}
51	3-Methyl-1-pentanol	589–35-5	C6H14O	329.788	856.0	1.5870	6.33 ± 4.93^{c}	7.67 ± 1.53^{c}	8.67 ± 0.58^{c}	47.00 ± 2.65^{b}	426.33 ± 12.90^{a}
52	trans-3-Hexen-1-ol	928–97-2	C6H12O	355.491	871.9	1.5395	38.33 ± 4.16^{c}	17.33 ± 2.08^{d}	20.00 ± 3.00^{d}	45.67 ± 1.15^{b}	338.33 ± 4.93^{a}
62	beta-Citronellol	106–22-9	C10H20O	1147.549	1275.4	1.3464	10.00 ± 3.46^{b}	5.00 ± 1.73^{bc}	1.67 ± 0.58^{c}	7.33 ± 0.58^{b}	242.00 ± 5.29^{a}
66	Nerol	106–25-2	C10H18O	1038.505	1217.0	1.7673	8.00 ± 1.73^{b}	7.67 ± 2.08^{b}	7.33 ± 0.58^{b}	7.33 ± 0.58^{b}	87.33 ± 7.37^{a}
67	Maltol	118–71–8	C6H6O3	894.883	1140.2	1.5213	20.00 ± 0.00^{b}	9.67 ± 0.58^{b}	5.33 ± 1.15^{b}	7.33 ± 1.15^{b}	128.33 ± 19.43^{a}
69	2-Phenylethanol	60–12-8	C8H10O	894.602	1140.0	1.3007	37.67 ± 5.86^{b}	21.67 ± 3.79^{c}	11.00 ± 1.73^{d}	16.33 ± 2.08^{cd}	93.67 ± 5.69^{a}
75	1-Phenylethanol	98–85-1	C8H10O	685.706	1028.2	1.5564	31.33 ± 3.06^{b}	18.67 ± 0.58^{c}	11.33 ± 1.15^{d}	14.33 ± 1.15^{cd}	175.00 ± 7.55^{a}
78	3-Octanol	589–98-0	C8H18O	627.073	996.8	1.7528	3.33 ± 1.15^{c}	15.67 ± 1.15^{b}	9.00 ± 1.73^{bc}	14.67 ± 3.79^{b}	56.33 ± 11.93^{a}
80	2-Heptanol	543–49-7	C7H16O	428.037	909.3	1.7160	2.67 ± 2.89^{c}	3.00 ± 1.00^{c}	5.00 ± 1.73^{c}	10.33 ± 1.53^{b}	88.67 ± 1.53^{a}
82	cis-2-Penten-1-ol	1576–95-0	C5H10O	182.890	752.3	1.4378	149.00 ± 11.79^{b}	66.67 ± 4.93^{e}	82.67 ± 4.51^{d}	99.33 ± 3.79^{c}	507.00 ± 9.54^{a}
84	1-Pentanol	71–41-0	C5H12O	232.204	795.3	1.5014	102.33 ± 19.55^{c}	103.67 ± 3.51^{c}	306.67 ± 26.08^{b}	301.00 ± 10.15^{b}	1065.33 ± 7.37^{a}
88	5-Methylfurfuryl alcohol (M)	3857-25-8	C6H8O2	542.126	958.9	1.2511	133.33 ± 9.24^{c}	240.33 ± 9.29^{a}	230.67 ± 14.50^{a}	227.00 ± 7.00^{a}	165.00 ± 2.65^{b}
92	5-Methylfurfuryl alcohol (D)	3857-25-8	C6H8O2	573.239	972.5	1.5746	32.33 ± 5.86^{c}	44.00 ± 3.46^{b}	30.00 ± 1.00^{c}	23.67 ± 0.58^{d}	179.67 ± 0.58^{a}
90	2-Furanmethanethiol	98–02-2	C5H6OS	481.523	932.5	1.1150	280.00 ± 5.57^{a}	117.67 ± 6.35^{b}	129.00 ± 1.73^{b}	83.33 ± 22.37^{c}	32.33 ± 1.53^{d}
94	1-Propanethiol	107–03-9	C3H8S	52.326	594.6	1.1773	457.00 ± 33.15^{c}	839.00 ± 32.51^{a}	371.33 ± 13.28^{d}	765.67 ± 4.73^{b}	446.67 ± 45.62^{c}
97	3-Methyl-3-buten-1-ol (M)	763–32-6	C5H10O	125.685	699.5	1.2916	175.00 ± 17.35^{c}	181.00 ± 13.86^{c}	204.00 ± 6.08^{b}	189.00 ± 10.58^{bc}	424.00 ± 4.36^{a}
99	3-Methyl-3-buten-1-ol (D)	763–32-6	C5H10O	156.344	727.8	1.5077	165.00 ± 40.63^{b}	21.67 ± 2.08^{d}	21.33 ± 8.50^{d}	58.67 ± 2.89^{c}	393.00 ± 4.00^{a}
104	3-Methyl-2-butanol	598–75-4	C5H12O	112.635	685.5	1.2402	117.67 ± 5.13^{c}	196.67 ± 4.16^{b}	127.00 ± 6.08^{c}	243.33 ± 13.28^{a}	66.33 ± 1.15^{d}
41	2-Methyl-1-propanol	78–83-1	C4H10O	91.086	653.0	1.1785	112.33 ± 4.16^{d}	253.67 ± 2.08^{b}	206.33 ± 4.51^{c}	274.67 ± 12.86^{a}	102.00 ± 5.57^{d}
Aldehydes (17)											
3	cis-4-Heptenal	6728-31-0	C7H12O	382.915	889.0	1.6253	106.67 ± 34.12^{c}	112.00 ± 19.97^{c}	86.33 ± 17.47^{c}	379.33 ± 58.96^{a}	239.00 ± 1.00^{b}
10	3-Methylbutanal	590–86-3	C5H10O	91.699	653.9	1.3986	1529.00 ± 14.93^{a}	889.00 ± 43.31^{b}	488.00 ± 13.86^{c}	323.00 ± 58.97^{d}	472.00 ± 18.36^{c}
14	trans-2-Pentenal	1576-87-0	C5H8O	174.427	744.5	1.3964	229.33 ± 40.08^{a}	140.00 ± 7.81^{c}	148.33 ± 12.90^{bc}	181.33 ± 15.28^{b}	260.33 ± 2.89^{a}
27	3-Methyl-2-butenal	107–86-8	C5H8O	199.736	767.8	1.0990	111.33 ± 47.01^{a}	97.33 ± 12.70^{a}	76.67 ± 2.31^{a}	97.33 ± 5.03^{a}	32.33 ± 1.53^{b}

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Table 5 (*continued*)

IMS Code	VOCs	CAS	Formular	Retention time [*sec*]	Retention index*	Drift time [RIP relative]	Peak volume (a.u.)				
							WGSO	PSO	WSO	CSO	BGSO
39	2-Methylpropanal (M)	78–84-2	C4H8O	32.938	565.3	1.1132	2322.67 ± 44.74^{b}	2668.00 ± 32.23^{a}	1920.33 ± 38.59^{c}	2234.33 ± 28.04^{b}	1886.67 ± 109.81^{c}
37	2-Methylpropanal (D)	78–84-2	C4H8O	50.162	591.3	1.2775	575.33 ± 49.74^{a}	287.33 ± 11.06^{c}	177.33 ± 11.02^{d}	172.33 ± 11.93^{d}	385.33 ± 9.24^{b}
46	trans-2-Heptenal	18,829–55-5	C7H12O	531.726	954.4	1.6550	20.67 ± 2.08^{c}	249.00 ± 33.15^{b}	95.33 ± 5.86^{c}	37.00 ± 7.94^{c}	1488.33 ± 168.05^{a}
56	2,4-Heptadienal	5910-85-0	C7H10O	631.296	999.1	1.6159	13.67 ± 1.15^{bc}	16.33 ± 1.15^{b}	8.00 ± 0.00^{c}	15.33 ± 1.53^{b}	145.33 ± 8.08^{a}
60	2,4-Nonadienal	5910-87-2	C9H14O	1092.721	1246.0	1.9340	8.00 ± 0.00^{b}	8.33 ± 0.58^{b}	9.00 ± 0.00^{b}	9.00 ± 0.00^{b}	117.00 ± 15.10^{a}
64	Octanal	124–13-0	C8H16O	663.246	1016.2	1.4083	112.33 ± 14.36^{b}	63.67 ± 0.58^{c}	48.67 ± 2.08^{c}	62.33 ± 2.89^{c}	345.33 ± 48.95^{a}
70	Benzeneacetaldehyde	122–78-1	C8H8O	721.176	1047.2	1.2521	92.00 ± 5.00^{c}	86.67 ± 2.08^{c}	86.67 ± 9.02^{c}	141.67 ± 6.81^{b}	226.00 ± 6.08^{a}
77	4-Methylbenzaldehyde	104–87-0	C8H8O	771.420	1074.1	1.5835	30.67 ± 1.15^{b}	16.00 ± 2.65^{c}	9.00 ± 1.00^{d}	11.33 ± 1.15^{d}	95.67 ± 2.52^{a}
81	2,4-Hexadienal	142–83-6	C6H8O	469.135	927.2	1.4810	85.67 ± 14.47^{b}	45.67 ± 4.04^{c}	33.33 ± 2.31^{c}	85.67 ± 5.13^{b}	199.67 ± 32.65^{a}
85	trans-2-Hexenal	505–57-7	C6H10O	323.204	851.9	1.5109	89.33 ± 2.08^{b}	115.33 ± 2.31^{b}	45.33 ± 15.28^{b}	110.00 ± 5.57^{b}	1238.00 ± 78.94^{a}
101	Furfural	98–01-1	C5H4O2	295.235	834.5	1.0781	170.67 ± 46.11^{a}	105.67 ± 7.09^{b}	92.00 ± 1.00^{b}	110.00 ± 1.73^{b}	38.33 ± 3.21^{c}
102	Methacrolein	78–85-3	C4H6O	20.515	546.6	1.0495	718.67 ± 28.68^{a}	566.67 ± 10.79^{b}	699.33 ± 4.51^{a}	524.67 ± 5.51^{b}	459.67 ± 45.65^{c}
109	2-Methylpentanal	123–15-9	C6H12O	204.049	771.8	1.5662	465.00 ± 80.55^{a}	351.00 ± 12.00^{b}	255.67 ± 23.80^{c}	307.67 ± 12.10^{bc}	512.00 ± 8.00^{a}
Esters (29)											
5	Isopentyl formate	110–45-2	C6H12O2	251.861	807.5	1.2711	251.33 ± 54.52^{a}	279.67 ± 11.06^{a}	293.67 ± 13.32^{a}	277.33 ± 8.02^{a}	72.00 ± 4.36^{b}
7	Propyl acetate	109–60-4	C5H10O2	169.814	740.2	1.1555	218.00 ± 11.00^{b}	434.67 ± 32.13^{a}	212.00 ± 87.43^{b}	243.33 ± 35.56^{b}	69.67 ± 9.02^{c}
8	Butyl formate	592–84-7	C5H10O2	134.024	707.2	1.1942	228.67 ± 9.61^{c}	268.33 ± 7.64^{b}	342.33 ± 3.21^{a}	202.00 ± 12.17^{d}	50.33 ± 2.52^{e}
11	Methyl butyrate	623–42-7	C5H10O2	121.933	696.0	1.4157	1069.00 ± 19.92^{a}	485.67 ± 27.97^{c}	800.67 ± 29.19^{b}	316.33 ± 25.11^{d}	538.67 ± 44.56^{c}
19	Butyl butyrate	109–21–7	C8H16O2	625.655	996.1	1.3322	175.33 ± 11.72^{a}	92.00 ± 4.36^{c}	60.33 ± 1.15^{d}	120.00 ± 2.00^{b}	127.67 ± 16.29^{b}
29	alpha-Angelica lactone	591–12-8	C5H6O2	377.656	885.7	1.3556	572.00 ± 226.44^{a}	340.33 ± 85.23^{b}	131.00 ± 60.51^{b}	133.33 ± 9.61^{b}	125.67 ± 20.84^{b}
33	Methyl acetate	79–20-9	C3H6O2	47.451	587.2	1.1934	663.33 ± 20.13^{a}	446.33 ± 19.60^{c}	220.67 ± 4.04^{d}	506.67 ± 12.22^{b}	427.33 ± 15.04^{c}
45	Amyl acetate (M)	628–63-7	C7H14O2	400.919	897.4	1.3239	134.67 ± 10.07^{c}	187.00 ± 22.27^{b}	212.33 ± 18.77^{b}	382.67 ± 6.35^{a}	86.33 ± 2.52^{d}
47	Amyl acetate (D)	628–63-7	C7H14O2	429.745	910.0	1.7493	0.33 ± 0.58^{b}	0.67 ± 0.58^{b}	2.67 ± 1.53^{b}	4.00 ± 0.00^{b}	322.67 ± 4.51^{a}
49	Ethyl pentanoate	539–82-2	C7H14O2	421.178	906.3	1.6826	4.67 ± 3.79^{c}	3.67 ± 0.58^{c}	6.67 ± 1.15^{c}	29.67 ± 0.58^{b}	298.33 ± 10.97^{a}
57	Butyl pentanoate	591–68-4	C9H18O2	807.843	1093.6	1.9305	8.33 ± 2.08^{b}	8.67 ± 0.58^{b}	8.33 ± 0.58^{b}	10.00 ± 1.73^{b}	227.67 ± 3.06^{a}
59	Butyl hexanoate	626–82-4	C10H20O2	1025.627	1210.1	2.0425	11.33 ± 1.15^{b}	12.67 ± 0.58^{b}	13.00 ± 1.00^{b}	14.00 ± 1.00^{b}	606.33 ± 10.02^{a}
61	Ethyl caprylate	106–32-1	C10H20O2	1045.607	1220.8	1.4752	7.00 ± 0.00^{b}	4.33 ± 1.53^{b}	3.00 ± 0.00^{b}	4.67 ± 1.15^{b}	311.00 ± 16.52^{a}
65	Pentyl butanoate	540–18-1	C9H18O2	836.366	1108.8	1.4103	37.67 ± 4.93^{b}	29.33 ± 0.58^{c}	28.33 ± 0.58^{c}	30.67 ± 1.15^{bc}	170.00 ± 7.55^{a}
68	3-Methylbutyl pentanoate	2050-09-1	C10H20O2	892.911	1139.1	1.4856	32.33 ± 3.21^{b}	18.67 ± 0.58^{cd}	15.67 ± 1.15^{d}	21.67 ± 1.15^{c}	103.00 ± 4.36^{a}
71	gamma-Heptalactone	105–21-5	C7H12O2	906.264	1146.3	1.2561	60.00 ± 6.08^{b}	33.33 ± 3.06^{c}	20.67 ± 2.08^{d}	24.00 ± 1.73^{d}	273.33 ± 6.51^{a}
72	Methyl 2-furoate	611–13-2	C6H6O3	582.395	976.5	1.4772	89.33 ± 12.42^{b}	53.00 ± 14.80^{bc}	33.33 ± 1.15^{c}	54.00 ± 3.46^{bc}	322.00 ± 47.47^{a}
76	Methyl 3-(methylthio) propionate	13,532–18-8	C5H10O2S	719.010	1046.0	1.5880	39.67 ± 2.52^{b}	19.33 ± 1.15^{c}	12.33 ± 0.58^{d}	14.33 ± 0.58^{cd}	114.67 ± 6.81^{a}
79	Ethyl 2-methylpentanoate	39,255–32-8	C8H16O2	519.015	948.9	1.7402	0.67 ± 1.15^{c}	2.67 ± 1.15^{b}	3.67 ± 0.58^{b}	4.33 ± 1.53^{b}	72.33 ± 0.58^{a}
86	Methyl 2-methylpropanoate	547–63-7	C5H10O2	118.648	693.0	1.4337	190.00 ± 30.12^{c}	321.33 ± 14.15^{b}	509.33 ± 6.81^{a}	223.33 ± 13.87^{c}	538.67 ± 44.56^{a}
91	Propyl propanoate	106–36-5	C6H12O2	242.946	801.9	1.5579	629.67 ± 104.21^{a}	521.00 ± 15.72^{b}	375.00 ± 41.07^{c}	455.00 ± 9.54^{bc}	482.67 ± 8.50^{b}
93	Methyl 2-methylbutyrate	868–57-5	C6H12O2	202.689	770.6	1.1847	142.00 ± 6.93^{a}	133.33 ± 7.51^{ab}	113.67 ± 5.51^{c}	126.00 ± 7.00^{b}	45.67 ± 2.52^{d}

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Table 5 (*continued*)

IMS Code	VOCs	CAS	Formular	Retention time [*sec*]	Retention index*	Drift time [RIP relative]	Peak volume (a.u.)				
							WGSO	PSO	WSO	CSO	BGSO
100	Ethyl propanoate	105–37-3	C5H10O2	150.151	722.1	1.4501	178.33 ± 35.92^{b}	32.00 ± 2.00^{c}	29.00 ± 3.46^{c}	42.00 ± 1.00^{c}	338.67 ± 13.32^{a}
107	Ethyl 2-methylbutyrate	7452–79-1	C7H14O2	282.829	826.7	1.2504	114.67 ± 9.45^{c}	101.00 ± 8.72^{d}	175.00 ± 6.00^{a}	154.67 ± 4.16^{b}	97.67 ± 4.51^{d}
110	Ethyl 2-hydroxypropanoate	97–64-3	C5H10O3	270.810	819.3	1.5211	49.33 ± 16.44^{b}	35.33 ± 0.58^{b}	36.00 ± 6.56^{b}	45.67 ± 0.58^{b}	470.00 ± 2.65^{a}
113	Ethyl formate	109–94-4	C3H6O2	58.366	603.7	1.2141	288.67 ± 6.81^{b}	263.33 ± 11.93^{c}	227.67 ± 3.51^{d}	596.00 ± 19.16^{a}	230.33 ± 2.52^{d}
117	Ethyl 2-methylpropanoate	97–62-1	C6H12O2	207.274	774.8	1.2033	144.00 ± 38.59^{a}	130.67 ± 9.81^{ab}	102.00 ± 4.58^{bc}	92.00 ± 3.00^{c}	39.00 ± 2.65^{d}
44	Ethyl crotonate	623–70-1	C6H10O2	285.862	828.6	1.1894	153.00 ± 19.05^{a}	137.33 ± 5.77^{b}	107.00 ± 5.20^{c}	108.00 ± 3.61^{c}	82.67 ± 20.03^{d}
89	Ethyl ethanoate	141–78-6	C4H8O2	83.960	642.2	1.1108	132.67 ± 1.53^{c}	221.33 ± 4.73^{b}	232.33 ± 2.89^{b}	275.67 ± 23.29^{a}	45.67 ± 3.21^{d}
Ketones (17)											
12	Cyclopentanone	120–92-3	C5H8O	241.208	800.9	1.3378	129.00 ± 19.08^{b}	163.00 ± 1.73^{a}	101.33 ± 11.37^{c}	156.67 ± 6.11^{a}	86.00 ± 9.17^{c}
21	3-Hepten-2-one	1119-44-4	C7H12O	450.917	919.2	1.2225	199.67 ± 103.00^{a}	153.33 ± 48.01^{ab}	75.00 ± 20.07^{b}	56.33 ± 0.58^{b}	69.33 ± 10.12^{b}
28	2-Methyltetrahydrofuran-3-one	3188-00-9	C5H8O2	206.450	774.0	1.0496	136.67 ± 64.70^{b}	157.33 ± 5.51^{b}	222.67 ± 14.43^{a}	149.67 ± 4.73^{b}	45.00 ± 6.24^{c}
31	Acetoin (M)	513–86-0	C4H8O2	170.151	740.5	1.0634	109.33 ± 19.60^{c}	184.00 ± 5.57^{a}	186.67 ± 6.81^{a}	133.67 ± 5.51^{b}	33.00 ± 1.73^{d}
112	Acetoin (D)	513–86-0	C4H8O2	164.932	735.7	1.3248	126.00 ± 30.51^{c}	180.33 ± 10.50^{b}	104.00 ± 2.00^{c}	217.00 ± 7.94^{a}	207.67 ± 5.03^{ab}
40	Hydroxyacetone	116–09-6	C3H6O2	72.178	624.5	1.0377	126.00 ± 3.46^{c}	161.33 ± 7.57^{b}	343.00 ± 1.73^{a}	169.67 ± 2.52^{b}	75.33 ± 10.12^{d}
54	2-Heptanone	110–43-0	C7H14O	476.040	885.2	1.6375	38.00 ± 1.73^{c}	64.00 ± 7.00^{b}	21.00 ± 7.21^{d}	29.33 ± 1.15^{cd}	298.67 ± 12.10^{a}
55	5-Methyl-2-hepten-4-one	81,925–81–7	C8H14O	563.059	968.1	1.7034	4.00 ± 2.00^{b}	12.67 ± 0.58^{b}	12.00 ± 0.00^{b}	10.00 ± 1.73^{b}	152.33 ± 22.48^{a}
58	2-Methyl-3-heptanone	13,019–20-0	C8H16O	810.902	1095.2	1.6869	8.33 ± 0.58^{b}	5.33 ± 1.15^{c}	6.67 ± 0.58^{bc}	7.33 ± 0.58^{bc}	131.00 ± 3.00^{a}
73	Cyclotene	80–71–7	C6H8O2	622.974	994.6	1.5370	55.00 ± 6.08^{cd}	108.00 ± 5.29^{b}	60.33 ± 14.05^{c}	31.33 ± 1.15^{d}	321.00 ± 29.05^{a}
87	Acetoxyacetone	592–20-1	C5H8O3	298.287	836.4	1.0494	200.67 ± 105.26^{a}	181.33 ± 16.92^{a}	228.67 ± 14.64^{a}	210.67 ± 5.69^{a}	45.67 ± 2.52^{b}
95	Butane-2,3-dione	431–03-8	C4H6O2	38.771	574.1	1.1747	514.67 ± 26.76^{b}	474.00 ± 8.00^{c}	280.33 ± 3.06^{d}	628.67 ± 5.51^{a}	499.33 ± 20.21^{bc}
106	3-Pentanone	96–22-0	C5H10O	102.795	670.6	1.3675	578.00 ± 24.88^{a}	369.00 ± 18.68^{c}	127.33 ± 4.73^{d}	153.00 ± 10.15^{d}	479.67 ± 75.29^{b}
108	3-Oxocyclohexene	930–68-7	C6H8O	399.926	897.0	1.4155	211.00 ± 43.41^{a}	42.33 ± 2.52^{b}	37.67 ± 1.15^{b}	72.33 ± 0.58^{b}	176.33 ± 17.95^{a}
111	Tetrahydrothiophen-3-one	1003-04-9	C4H6OS	475.625	930.0	1.4186	287.00 ± 26.00^{a}	86.33 ± 4.93^{c}	54.33 ± 13.05^{d}	52.67 ± 4.16^{d}	184.33 ± 6.43^{b}
98	1-Pentene-3-one (M)	1629-58-9	C5H8O	87.719	647.9	1.2889	200.00 ± 23.07^{b}	178.67 ± 9.07^{bc}	171.67 ± 3.21^{c}	175.33 ± 8.50^{c}	412.00 ± 8.72^{a}
36	1-Pentene-3-one (D)	1629-58-9	C5H8O	99.794	666.1	1.3062	226.33 ± 8.02^{b}	185.00 ± 2.00^{c}	112.67 ± 4.04^{e}	122.00 ± 5.29^{d}	251.00 ± 1.73^{a}
Ethers (3)											
23	2-Butoxyethanol (M)	111–76-2	C6H14O2	397.817	896.1	1.1981	155.00 ± 8.72^{a}	134.33 ± 5.77^{b}	77.67 ± 7.23^{d}	64.00 ± 1.00^{e}	111.67 ± 2.31^{c}
48	2-Butoxyethanol (D)	111–76-2	C6H14O2	440.810	914.8	1.6603	4.00 ± 3.46^{c}	2.67 ± 0.58^{c}	4.33 ± 1.53^{c}	74.00 ± 9.00^{b}	438.00 ± 5.57^{a}
43	2-Ethoxyethanol	110–80-5	C4H10O2	146.909	719.1	1.0875	63.00 ± 11.53^{c}	93.00 ± 6.08^{b}	90.33 ± 0.58^{b}	150.67 ± 7.51^{a}	30.00 ± 0.00^{d}
Acids (9)											
15	Butanoic acid	107–92-6	C4H8O2	226.471	791.7	1.4024	204.67 ± 8.50^{a}	164.33 ± 15.95^{b}	204.67 ± 24.83^{a}	170.00 ± 7.00^{b}	168.00 ± 1.00^{b}
22	Isovaleric acid	503–74-2	C5H10O2	332.290	857.5	1.2218	183.67 ± 92.12^{a}	122.67 ± 36.91^{ab}	64.00 ± 7.94^{b}	64.67 ± 2.08^{b}	50.67 ± 5.51^{b}
35	Caproic acid	142–62-1	C6H12O2	693.983	1032.6	1.2975	125.00 ± 9.54^{a}	49.33 ± 4.04^{c}	54.33 ± 3.51^{c}	50.33 ± 3.06^{c}	109.67 ± 1.15^{b}
50	2-Methylpentanoic acid	97–61-0	C6H12O2	494.581	938.2	1.5764	20.67 ± 2.08^{bc}	25.67 ± 3.79^{b}	15.00 ± 2.65^{c}	17.67 ± 1.15^{c}	234.33 ± 5.13^{a}
63	Octanoic acid	124–07-2	C8H16O2	981.627	1186.6	1.4204	16.33 ± 2.89^{b}	10.00 ± 2.00^{b}	8.00 ± 0.00^{b}	10.33 ± 1.53^{b}	202.33 ± 9.71^{a}
74	2-Methylbutanoic acid	116–53-0	C5H10O2	300.578	837.8	1.4792	35.00 ± 20.95^{b}	32.67 ± 1.15^{b}	32.67 ± 2.31^{b}	39.00 ± 2.65^{b}	665.00 ± 17.32^{a}
83	Propanoic acid	79–09-4	C3H6O2	155.177	726.7	1.3516	129.33 ± 31.50^{b}	99.00 ± 6.56^{bc}	54.67 ± 3.21^{c}	152.00 ± 7.00^{b}	411.00 ± 67.62^{a}
116	Pentanoic acid	109–52-4	C5H10O2	383.670	889.5	1.5033	200.33 ± 4.93^{b}	166.00 ± 2.65^{b}	69.00 ± 21.63^{c}	102.00 ± 4.00^{c}	391.67 ± 52.35^{a}

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Table 5 (*continued*)

IMS Code	VOCs	CAS	Formular	Retention time [*sec*]	Retention index*	Drift time [RIP relative]	Peak volume (a.u.)				
							WGSO	PSO	WSO	CSO	BGSO
118	Crotonic acid	107–93-7	C4H6O2	274.912	821.8	1.1022	140.33 ± 4.51^{a}	106.67 ± 7.37^{b}	68.67 ± 5.03^{c}	104.67 ± 4.16^{b}	37.67 ± 2.89^{d}
Others (12)											
24	trans-beta-Ocimene	13,877–91-3	C10H16	723.352	1048.4	1.2235	170.33 ± 45.36^{a}	157.00 ± 16.52^{a}	73.00 ± 24.02^{b}	74.33 ± 1.15^{b}	96.00 ± 13.08^{b}
9	3-Butenenitrile	109–75-1	C4H5N	90.370	651.9	1.2572	298.00 ± 73.43^{a}	341.33 ± 11.93^{a}	149.67 ± 1.53^{b}	324.00 ± 8.19^{a}	207.00 ± 4.58^{b}
114	Hexanenitrile	628–73-9	C6H11N	376.641	885.1	1.5790	24.00 ± 6.08^{c}	19.67 ± 4.16^{c}	28.33 ± 7.02^{c}	62.67 ± 1.53^{b}	343.33 ± 31.07^{a}
6	Pyridine	110–86-1	C5H5N	209.731	777.1	1.2502	192.33 ± 8.08^{d}	222.67 ± 7.77^{c}	358.33 ± 17.47^{a}	315.67 ± 2.52^{b}	52.67 ± 7.64^{e}
105	2,6-Dimethylpyridine	108–48-5	C7H9N	361.548	875.7	1.4474	56.00 ± 2.00^{b}	51.67 ± 2.08^{b}	41.67 ± 3.06^{b}	68.33 ± 0.58^{b}	178.67 ± 31.72^{a}
115	3-Ethylpyridine	536–78-7	C7H9N	548.977	961.9	1.5204	83.67 ± 3.21^{c}	175.67 ± 4.04^{b}	91.33 ± 20.60^{c}	53.33 ± 3.21^{d}	290.33 ± 27.61^{a}
53	2,6-Dimethylpyrazine	108–50-9	C6H8N2	449.979	918.8	1.5643	23.33 ± 2.52^{b}	8.33 ± 0.58^{c}	9.67 ± 2.08^{c}	23.00 ± 2.65^{b}	412.00 ± 9.64^{a}
103	Pyrrolidine	123–75-1	C4H9N	129.516	703.0	1.2663	153.00 ± 2.00^{d}	222.67 ± 4.04^{b}	133.00 ± 4.00^{e}	244.67 ± 4.04^{a}	166.00 ± 3.00^{c}
32	Tetrahydrofuran	109–99-9	C4H8O	57.914	603.0	1.2397	1031.67 ± 100.72^{a}	914.00 ± 21.70^{ab}	300.67 ± 12.86^{d}	449.33 ± 11.15^{c}	861.67 ± 119.07^{b}
18	2,2,4,6,6-Pentamethylheptane	13,475–82-6	C12H26	631.768	999.3	1.3577	193.67 ± 3.21^{a}	125.67 ± 3.51^{b}	67.67 ± 22.72^{c}	66.67 ± 2.52^{c}	204.33 ± 23.46^{a}
30	Diethyl acetal	105–57-7	C6H14O2	159.128	730.3	1.0399	138.00 ± 45.74^{c}	173.00 ± 1.00^{c}	285.00 ± 23.81^{a}	223.33 ± 1.53^{b}	36.33 ± 3.21^{d}
34	2-Octanol	123–96-6	C8H18O	669.954	1019.8	1.4527	162.67 ± 15.37^{a}	36.33 ± 8.39^{b}	18.67 ± 1.15^{c}	24.33 ± 1.15^{bc}	148.00 ± 10.82^{a}

(M), monomer; (D), dimer;

* Retention index was calculated refereed to the retention time of C4–C9 n-ketones under the same conditions;

^{a,b,c,d,e} Values in the same row with different letters are significant difference at $p < 0.05$, results are expressed as mean ± standard deviation (n = 3).

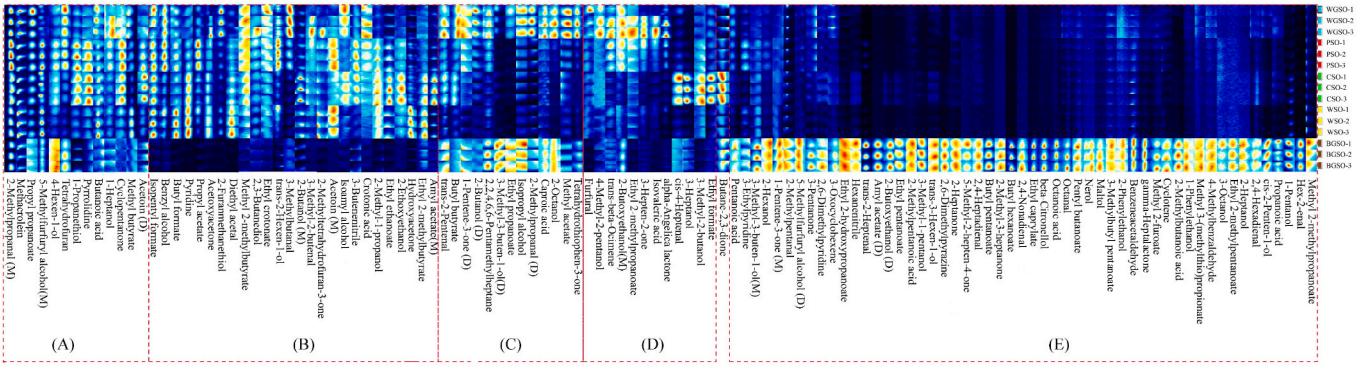

Fig. 1. VOC fingerprints of five Cucurbitaceae seed oils by HS-GC–IMS. The redder the area, the higher the signal intensity of VOCs. Each row represents all the signals from one sample. Each column represents the signals of the same VOC. (M) and (D) denote monomer and dimer, respectively.

2022). Additionally, high concentrations of hexanal, nonanal, and 2-nonenal have also been reported to be key aroma components in cucumber fruits (Shan et al., 2020). BGSO has the fewest aldehydes detected but the highest overall content, mainly due to the high levels of 2,4-nonadienal, 10-undecenal, and trans-2-hexenal. 2,4-Nonadienal is known as a compound originating from the oxidation of linolenic acid (Zhang et al., 2021). It is also reported as the key odorant with the highest odor activity values in rapeseed oil, which contributes to deep-fried, fatty, green aromas (Pollner & Schieberle, 2016). Furthermore, trans-2-hexenal has been reported as one of the main volatile components in the fruits and vines of bitter gourd (Binder et al., 1989). WGSO also contained high levels of aldehydes, with benzaldehyde and 2,4-decadienal being prominent. Additionally, nonanal (green, fatty, and soapy aromas) and decanal (green and nutty aromas) have been reported as important aroma components in the volatile oil of wax gourd (Sharma et al., 2010). PSO and WSO contained low content of aldehydes, mainly including heptenal and nonanal, which were the main volatile aldehydes in roasted pumpkin seeds and produced PSO (exceeding 10,000 ppb) (Bowman et al., 2012). Their content showed very large increases in concentrations during the roasting process (Siegmund et al., 2004). The aldehydes with high concentrations in WSO include trans-2-heptenal, benzaldehyde, nonanal, etc., some of which have been reported in the literature (Ok & Yilmaz, 2019).

HS-SPME-GC–MS identified only six ketones in the five seed oils, and their species and content in each oil sample were significantly different. Ketones are typically found in low concentrations in Cucurbitaceae seed oils, intensifying the slightly fruity attributes (Moronkola et al., 2009; Siegmund & Murkovic, 2004). BGSO exhibited the highest content of ketones detected, with 5-decanone and 7-dodecen-6-one having the highest abundance. In contrast, WGSO contained a high concentration of 3-octen-2-one. Furthermore, a considerable number of heterocyclic compounds, such as pyrazines, pyrroles, pyridines, and furans, were also

Table 6
The composition and concentration of VOCs identified in three samples using HS-SPME-GC–MS.

Codes	Time (min)	Volatile compounds	Formula	CAS	RI Cal *	RI Ref #	Concentration (mg/kg)				
							WGSO	PSO	WSO	CSO	BGSO
		Alcohols (18)									
1’	3.95	Isoamyl alcohol	C5H12O	123–51-3	731	732					6.93 ± 0.68
2’	4.54	1-Pentanol	C5H12O	71–41-0	765	764					287.29 ± 9.98
3’	4.99	2,3-butanediol	C4H10O2	513–85-9	790	782	15.99 ± 1.87				
5’	5.17	3-Methyl-2-pentanol	C6H14O	565–60-6	800	797		6.43 ± 0.54			
8’	6.98	1-Hexanol	C6H14O	111–27-3	867	865	1.93 ± 0.19^{d}	5.16 ± 0.09^{c}	2.27 ± 0.14^{d}	31.27 ± 1.60^{a}	24.76 ± 0.52^{b}
11’	9.33	3-Hepten-1-ol	C7H14O	10,606–47-0	947	940					30.52 ± 0.66
13’	9.58	2-methylidenecyclohexan-1-ol	C7H12O	4065-80-9	956	974					49.12 ± 2.56
15’	9.98	cis-2-Methylcyclohexanol	C7H14O	7443-70-1	969	946					30.95 ± 1.34
16’	10.29	1-Octen-3-ol	C8H16O	3391–86-4	979	979		3.79 ± 0.21^{a}	2.68 ± 0.24^{b}		
24’	11.92	Benzyl alcohol	C7H8O	100–51-6	1031	1032	12.29 ± 0.70^{a}		1.71 ± 0.16^{c}	4.46 ± 0.19^{b}	2.24 ± 0.30^{c}
27’	12.15	2,6-Dimethylheptan-4-ol	C9H20O	108–82-7	1039						36.25 ± 0.82
30’	12.72	1-Octyn-3-ol	C8H14O	818–72-4	1057						5.08 ± 0.34
33’	13.00	trans-2-Octen-1-Ol	C8H16O	18,409–17-1	1066	1069					3.19 ± 0.05
36’	13.70	2,6-Dimethylheptan-4-ol	C9H20O	108–82-7	1089						2.18 ± 0.05
40’	14.30	2-Phenylethanol	C8H10O	60–12-8	1108	1110	22.93 ± 2.17^{b}	0.82 ± 0.10^{c}	0.68 ± 0.05^{c}	1.17 ± 0.12^{c}	25.90 ± 1.40^{a}
48’	16.02	1-Butyl-2-cyclohexen-1-ol	C10H18O	88,116–46-5	1165						7.18 ± 1.00
56’	17.62	2,4-Nonadien-1-ol	C9H16O	64,576–90-5	1220	1175					87.31 ± 4.25
58’	18.93	4-Methyl-5-thiazoleethanol	C6H9NOS	137–00-8	1266	1258	2.69 ± 0.58				
		Aldehydes (16)									
4’	5.15	Hexanal	C6H12O	66–25-1	799	802				1.84 ± 0.11	
7’	6.58	trans-2-Hexenal	C6H10O	6728-26-3	852	857					10.34 ± 0.25
12’	9.57	trans-2-Heptenal	C7H12O	18,829–55-5	955	960		11.72 ± 0.31^{a}	5.19 ± 0.23^{b}		
14’	9.66	Benzaldehyde	C7H6O	100–52-7	958	960	18.35 ± 1.04^{a}		1.37 ± 0.22^{c}	6.04 ± 1.05^{b}	
21’	11.43	2,4,6-Octatrienal	C8H10O	17,609–31-3	1015	1029					3.62 ± 0.08
28’	12.24	Benzeneacetaldehyde	C8H8O	122–78-1	1042	1043	3.24 ± 0.16^{a}		0.17 ± 0.02^{b}	0.24 ± 0.06^{b}	
39’	14.12	Nonanal	C9H18O	124–19-6	1102	1104	6.63 ± 0.33^{a}	2.95 ± 0.17^{c}	1.80 ± 0.18^{d}	1.92 ± 0.14^{d}	4.55 ± 0.47^{b}
44’	15.75	2-Nonenal	C9H16O	18,829–56-6	1156	1155	2.60 ± 0.36^{a}			1.50 ± 0.16^{b}	
45’	15.82	10-Undecenal	C11H20O	112–45-8	1159	1279					11.82 ± 0.38
46’	15.83	4-Ethylbenzaldehyde	C9H10O	4748-78-1	1159	1171		0.67 ± 0.04^{a}	0.70 ± 0.14^{a}	0.59 ± 0.02^{a}	
53’	16.84	2,4-Nonadienal	C9H14O	5910-87-2	1193	1195					31.76 ± 1.76
54’	17.11	Decanal	C10H20O	112–31-2	1202	1203	2.94 ± 0.24^{a}			0.28 ± 0.05^{b}	
55’	17.35	2,6-Dimethylbenzaldehyde	C9H10O	1123-56-4	1210	1208			0.82 ± 0.29^{b}	2.39 ± 0.16^{a}	
57’	18.45	4-Methoxybenzaldehyde	C8H8O2	123–11-5	1249	1252	4.47 ± 0.36				
59’	20.23	2,4-Decadienal	C10H16O	25,152–84-5	1312	1317	10.08 ± 0.88^{a}		0.72 ± 0.11^{b}	0.46 ± 0.03^{b}	
62’	22.19	Vanillin	C8H8O3	121–33-5	1385	1394	4.07 ± 0.19^{a}			0.22 ± 0.01^{b}	
		Esters (5)									
38’	13.81	Pentyl valerate	C10H20O2	2173-56-0	1092	1155					67.86 ± 3.28
42’	15.44	γ-Heptalactone	C7H12O2	105–21-5	1146	1130					9.49 ± 0.41
43’	15.59	3-Methylbutyl pentanoate	C10H20O2	2050-09-1	1151	1152					12.54 ± 0.89
61’	21.31	γ-nonalactone	C9H16O2	104–61-0	1352	1350				0.88 ± 0.04	
65’	25.86	Phenethyl 2-methylbutyrate	C13H18O2	24,817–51–4	1533	1493					0.34 ± 0.05
		Ketones (6)									
22’	11.64	2-Octen-4-one	C8H14O	4643-27-0	1022						5.10 ± 0.21
26’	12.06	3-Octen-2-one	C8H14O	1669-44-9	1036	1040	9.42 ± 0.66^{a}			2.28 ± 0.11^{b}	

(*continued on next page*)

Table 6 (*continued*)

Codes	Time (min)	Volatile compounds	Formula	CAS	RI Cal *	RI Ref #	Concentration (mg/kg)				
							WGSO	PSO	WSO	CSO	BGSO
37’	13.76	3,5-Octadien-2-one	C8H12O	38,284–27-4	1091	1092		1.94 ± 0.21[a]	0.86 ± 0.08[b]		
49’	16.11	5-Decanone	C10H20O	820–29-1	1168	1162					18.77 ± 1.52
60’	20.27	7-Dodecen-6-one	C12H22O	32,064–76-9	1313						14.07 ± 0.65
64’	24.36	β-Ionone	C13H20O	79–77-6	1471	1475					1.20 ± 0.06
		Acids (3)									
6’	6.47	2-Methylbutanoic acid	C5H10O2	116–53-0	848	854	2.39 ± 0.17				
18’	10.70	Caproic Acid	C6H12O2	142–62-1	992	990					40.79 ± 1.80
47’	15.94	Octanoic acid	C8H16O2	124–07-2	1163	1169	1.45 ± 0.38				
		Pyrazine (4)									
10’	8.16	2,5-Dimethylpyrazine	C6H8N2	123–32-0	909	915	20.67 ± 1.41[a]	8.74 ± 0.03[b]	4.99 ± 0.35[c]	1.38 ± 0.09[d]	
19’	10.92	2,3,5-Trimethylpyrazine	C7H10N2	14,667–55-1	999	1005	24.99 ± 1.50[a]	9.98 ± 0.35[b]	7.04 ± 1.05[c]		
34’	13.20	2,6-Diethylpyrazine	C8H12N2	13,067–27-1	1073	1081	13.68 ± 1.16[a]	1.96 ± 0.11[b]	0.60 ± 0.06[c]	0.53 ± 0.12[c]	
50’	16.22	2-Isobutyl-3-methoxypyrazine	C9H14N2O	24,683–00-9	1172	1179					2.93 ± 0.02
		Phenol (1)									
52’	16.54	2-Methoxy-4-methylphenol	C8H10O2	93–51-6	1183	1181	7.10 ± 0.49				
		Others (13)									
9’	7.58	Styrene	C8H8	100–42-5	889	895	1.58 ± 0.20[c]	2.38 ± 0.13[b]	0.80 ± 0.13[d]	9.07 ± 0.31[a]	
17’	10.59	2-Pentylfuran	C9H14O	3777–69-3	988	993	3.82 ± 0.43[c]	5.00 ± 0.24[b]		13.75 ± 0.72[a]	
20’	11.03	2-Propylthiophene	C7H10S	1551-27-5	1003	966					1.93 ± 1.46
23’	11.65	p-Cymene	C10H14	99–87-6	1023	1028				1.64 ± 0.09	
25’	11.99	Methacrylic anhydride	C8H10O3	760–93-0	1034	1054		6.84 ± 0.31			
29’	12.56	2-(2-Pentenyl)furan	C9H12O	70,424–14-5	1052	1048					4.76 ± 0.31
31’	12.73	2-Acetylpyrrole	C6H7NO	1072-83-9	1057	1059	11.84 ± 1.15				
32’	12.92	2-Pyrrolidinone	C4H7NO	616–45-5	1064	1076	18.40 ± 1.62				
35’	13.47	4-Allyltoluene	C10H12	3333-13-9	1081	1096		1.33 ± 0.22[a]	1.19 ± 0.31[a]	1.45 ± 0.05[a]	
41’	14.58	3-Pyridinemethanol	C6H7NO	100–55-0	1118	1119	1.30 ± 0.17				
51’	16.46	Naphthalene	C10H8	91–20-3	1180	1181	2.14 ± 0.42[b]	4.02 ± 0.10[a]	1.46 ± 0.51[c]	1.91 ± 0.05[bc]	
63’	22.41	Tetradecane	C14H30	629–59-4	1393	1400	1.52 ± 0.11[a]		1.47 ± 0.14[a]	1.29 ± 0.03[b]	
66’	26.36	α-Farnesene	C15H24	502–61–4	1555	1524					27.40 ± 0.80

* RI cal, retention index (Kovats RI), which was calculated refereed to the retention time of C5-C30 n-alkanes under the same conditions.
# RI ref., retention index was obtained from NIST Standard Reference Database (https://webbook.nist.gov/chemistry/).
[a,b,c,d] Values in the same row with different letters are significant difference at $p < 0.05$, results are expressed as mean ± standard deviation (n = 3).

detected in the oil samples, especially in WGSO. These compounds are generated during the Maillard reaction in many heat-processed foods and are often responsible for their roasted aroma. Heterocyclic compounds positively correlate with applied heating temperature and time (Zhang et al., 2021). Pyrazines, including 2,5-dimethylpyrazine, 2,3,5-trimethylpyrazine, and 2,6-diethylpyrazine, were most abundant in WGSO and PSO. These results are consistent with previous studies that abundant pyrazine derivatives were detected in WGSO and PSO, which can contribute to the roasted and nutty aromas (Ok et al., 2019; Siegmund et al., 2004). Additionally, higher concentrations of 2-acetylpyrrole and 2-pyrrolidinone were detected in WGSO. CSO contained higher concentrations of styrene and 2-pentylfuran. Moreover, the high content of caproic acid and α-farnesene in BGSO should also be noted, as these two VOCs can contribute sweet and wood aromas with extremely low odor thresholds (Qin et al., 2023), possibly being the main contributors to the unique woody floral sweetness of BGSO.

The detected varieties and contents of VOCs were consistent with the reported results of Cucurbitaceae fruits and seed oils (Mi et al., 2022; Ok et al., 2019). Notably, twelve common VOCs were detected by both methods, including benzyl alcohol, isoamyl alcohol, 2-phenylethanol, trans-2-heptenal, 2,4-nonadienal, benzeneacetaldehyde, 3-methylbutyl pentanoate, gamma-heptalactone, caproic acid, octanoic acid, 2-methylbutanoic acid, and 2,6-dimethylpyrazine. These compounds belong to the higher boiling point substances among all the detected VOCs, which also demonstrates the detection range differences between HS-SPME-GC–MS and HS-GC–IMS. Specifically, the strong ability of SPME to trap high-boiling compounds naturally contributed to a higher content of high-boiling compounds among the VOCs detected by HS-SPME-GC–MS, such as benzene derivatives and heterocyclic compounds (Ma et al., 2023). Overall, HS-GC–IMS can serve as a great complement to HS-SPME-GC–MS analysis in food VOC analysis.

3.7. PCA of volatile profiles by HS-GC–IMS and HS-SPME-GC–MS

To better analyze the differences of the VOC profiles of the five seed oils in an untargeted manner, an unsupervised PCA method was employed. PCA is an unsupervised clustering method that decreases the dimensionality of multivariate data (Ma et al., 2023). Fig. 2A and C show the PCA score plots of HS-GC–IMS and HS-SPME-GC–MS volatile profiles, respectively. The first two principal components of HS-GC–IMS

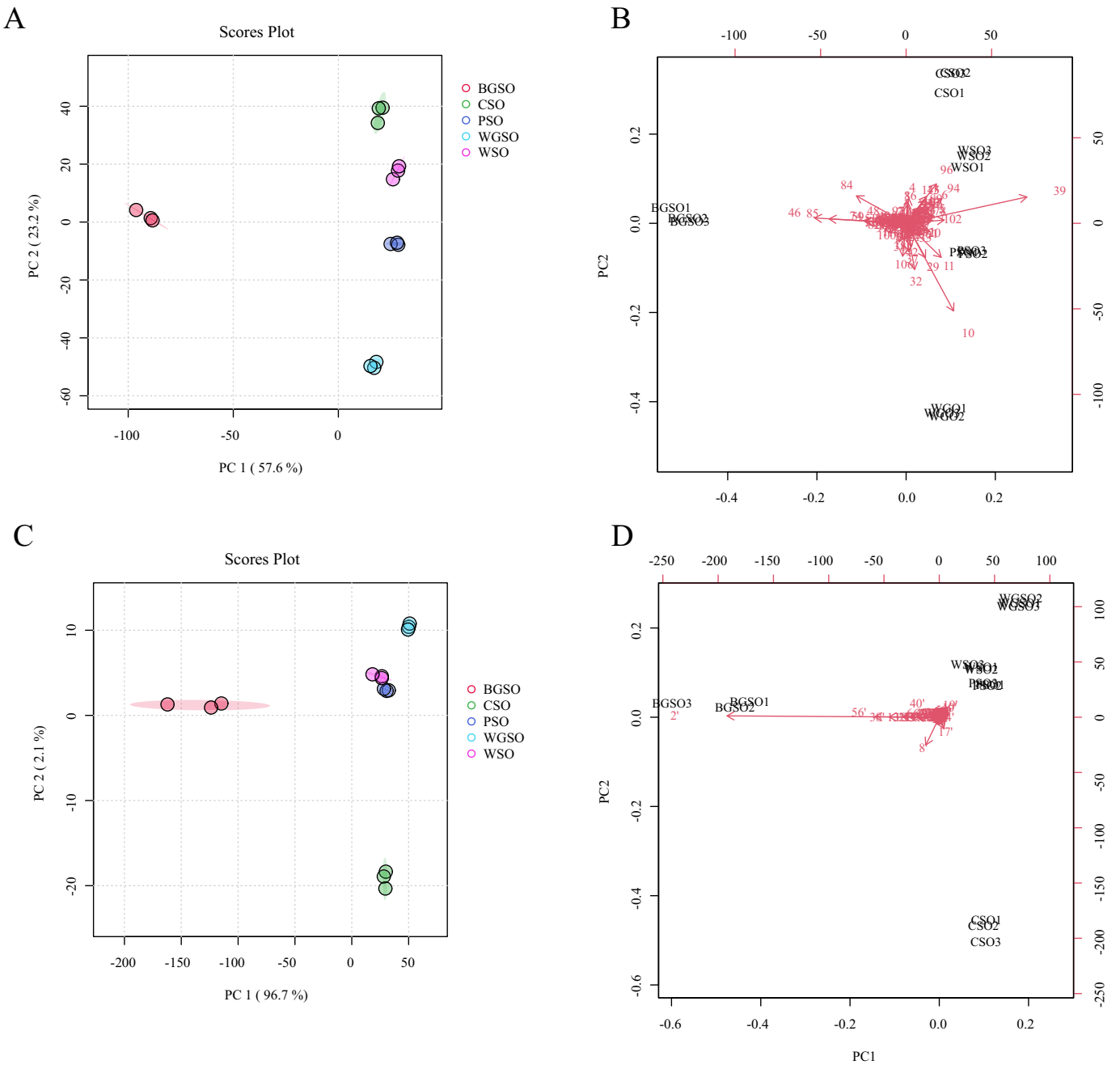

Fig. 2. Principal component analysis (PCA) of volatile profiles by HS-GC–IMS and HS-SPME-GC–MS. (A) & (C) The PCA scores plots and biplots based on HS-GC–IMS, the compound code corresponds to Table 5. (B) & (D) The PCA scores plots and biplots based on HS-SPME-GC–MS, the compound code corresponds to Table 6.

and HS-SPME-GC–MS explained 80.8 % and 98.8 % of the total variance, respectively. The PCA score plots clearly separated the five samples into uncorrelated sections, indicating significant differences in their volatile profiles. Notably, BGSO segregated in the left negative PC1 area, apart from other four seed oils clustered in the right positive PC1 area. These results correspond with the HS-GC–IMS fingerprint and TIC of HS-SPME-GC–MS, indicating that BGSO has a distinct VOC composition. By contrast, the PCA model of HS-GC-IMS is more effective in differentiating samples, especially along PC2, which explains 23.2 % of the total variance without overlap. PCA biplots were generated to show how variables affected the sample scattering behavior. HS-GC–IMS model (Fig. 2B) showed high loadings of trans-2-heptenal (46), trans-2-hexenal (85), 1-pentanol (84), 2-butoxyethanol (D) (48), 2-methylpropanal (M) (39), 3-methylbutanal (10), 2-butanol (M) (96), 1-propanethiol (94), methacrolein (102), methyl butyrate (11), alpha-angelica lactone (29), tetrahydrofuran (32), and 3-methylbutanal (10). These VOCs contributed most to the segregation of the five samples. Similarly, 1-pentanol (2'), 2,4-nonadien-1-ol (56'), pentyl valerate (38'), 2-phenylethanol (40'), 1-hexanol (8'), nonanal (39'), styrene (9'), and 2-pentylfuran (17') were key compounds influencing sample segregation in HS-SPME-GC–MS results (Fig. 2D).

4. Conclusions

The physicochemical properties of these seed oils were in accordance with official standards. PSO exhibited the highest oil yield, while BGSO had the highest total phenolic content. The mineral profiles are consistent with relevant literature, reflecting the influence of environmental

and biological factors. Linoleic acid was the dominant fatty acid in WSO, PSO, WGSO, and CSO, making up over 65 % of the total fatty acid content, except in PSO where it constituted 47.49 %. In contrast, α-eleostearic acid was the primary component in BGSO, accounting for 55.38 % of its fatty acids. All the seed oils are rich in tocopherols and squalene, their concentrations vary significantly. WSO had the highest total tocopherol content (1476.39 mg/kg), predominantly in the form of δ-tocopherol. PSO had the highest squalene content (1511.74 mg/kg), suggesting potential industrial applications. These variations highlight the impact of seed type and cultivation conditions on bioactive compounds. A total of 118 VOCs were identified in five seed oils using HS-GC–IMS, with significant differences observed in their VOC fingerprints. HS-SPME-GC–MS results were consistent with HS-GC–IMS, though the former detected fewer VOCs due to methodological differences. BGSO exhibited the most distinct volatile characteristics, rich in aliphatic alcohols and esters. Furthermore, PCA models effectively segregated the seed oils based on volatile profiles, confirming their VOC differences. These findings offer valuable insights for developing premium edible oils and dietary supplements. Future research will explore the impact of various roasting conditions on the aroma of Cucurbitaceae seed oils, as roasting can significantly modify their volatile profiles and improve their overall aroma.

CRediT authorship contribution statement

Pengfei Han: Validation, Investigation. **Jiawei Cheng:** Validation, Investigation. **Jingyi Wang:** Methodology. **Jingren He:** Methodology, Conceptualization. **Rui Zhang:** Methodology, Funding acquisition. **Muci Wu:** Writing – review & editing, Writing – original draft, Supervision, Funding acquisition. **Yin Xiong:** Funding acquisition.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.fochx.2024.101816.

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