



Comparative GC-MS Profiling of Chemical Constituents in Fresh and Dried Tomato (*Solanum lycopersicum* L.) at Different Drying Temperatures

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ABSTRACT :

Tomato (*Solanum lycopersicum* L.) is highly perishable, and drying can modify its detectable chemical profile through moisture removal, matrix disruption, changes in extractability, and heat-associated reactions. This study compared the GC-MS profiles of fresh tomato with samples dried at 40, 50, and 60 °C. Ethanol extracts were examined with a Shimadzu GCMS-QP2010 Plus instrument, and detected signals were assigned tentatively through comparison with a mass-spectral library. Relative peak-area normalization was applied to describe the contribution of individual signals within each chromatogram. The original instrument records contained 13 peaks for fresh tomato, 20 at 40 °C, 25 at 50 °C, and 26 at 60 °C. After repeated library names were consolidated, 59 different tentative compound labels were represented across the four profiles. Five labels ferulic acid, n-hexadecanoic acid, naringenin, "Quertine," and lycopene showed non-zero values in every condition. In the fresh sample, the largest relative signals were assigned to ferulic acid (27.06%), n-hexadecanoic acid (25.73%), oleic acid (21.90%), and octadecanoic acid (6.98%). At 40 °C, Z-11-hexadecenoic acid accounted for 59.95% of the relative signal, while erucic acid (32.90%) was dominant at 50 °C and ethylene diacrylate (40.37%) was the leading library assignment at 60 °C. The relative signal for lycopene was greatest at 50 °C (9.43%). Shannon diversity values were 1.904, 1.582, 2.426, and 2.210 for fresh, 40, 50, and 60 °C samples, respectively. Jaccard similarity values ranged from 0.147 to 0.278, with the highest overlap between the 40 and 60 °C profiles. Bray-Curtis dissimilarity was greatest for fresh versus 60 °C (0.969), whereas the 40 and 60 °C profiles had the lowest dissimilarity (0.882; similarity 0.118). These observations indicate substantial temperature-associated differences in the detectable GC-MS fingerprints. Because only one profile represented each condition and the compound identities were obtained by library matching, the relative peak areas must not be interpreted as absolute concentrations or definitive evidence of compound formation. The results are therefore best viewed as a descriptive fingerprinting dataset that can guide future work involving replicated measurements, authentic standards, retention-index confirmation, and validated quantitative methods.

Keywords: tomato; *Solanum lycopersicum*; GC-MS; drying temperature; chemical fingerprint; lycopene; relative peak area; Jaccard similarity; Bray-Curtis dissimilarity.

1. Introduction

Tomato (*Solanum lycopersicum* L.) is widely consumed either fresh or after processing and provides a range of nutrients and phytochemicals, including vitamins, minerals, carotenoids and phenolic compounds. Among these constituents, lycopene is particularly important because it contributes strongly to tomato pigmentation and is associated with nutritional and processing quality. The chemical composition detected in tomato is not fixed; it can vary according to cultivar, maturity, handling after harvest, and the processing conditions applied (Ali *et al.*, 2021; Lima *et al.*, 2022; Bajon *et al.*, 2026).

The high moisture content of fresh tomato makes the fruit vulnerable to rapid deterioration. Drying is consequently used to lower water availability, reduce product volume and extend storage life. However, dehydration is not simply a moisture-removal operation. Changes in temperature and exposure time can modify the plant matrix and consequently influence the release, accessibility, retention and chromatographic response of phytochemicals. Research using solar, hot-air and related drying systems has reported changes in tomato colour, antioxidant properties, phytochemical composition and other quality characteristics in response to processing conditions (Al Maiman *et al.*, 2021; Degwale *et al.*, 2022; Mwendu *et al.*, 2018; Obadina *et al.*, 2018; Dufera *et al.*, 2021; Tan *et al.*, 2021; Correia *et al.*, 2015; Alemayehu *et al.*, 2026).

The response of tomato phytochemicals to drying temperature is therefore unlikely to follow a single pattern. Heat exposure may reduce compounds that are thermally unstable, while dehydration and disruption of the food matrix can also make some constituents more accessible to extraction or analysis. Previous studies have reported temperature- and time-dependent changes in vitamin C, phenolic compounds, carotenoids and related quality attributes, and reviews have described both apparent retention gains and losses during heating (Degwale *et al.*, 2022; ElGamal *et al.*, 2023; Lima *et al.*, 2022; Nzimande *et al.*, 2025; Pravitha *et al.*, 2024; Wu *et al.*, 2022). This interaction between degradation, concentration and extractability is important when interpreting GC-MS peak-area data because a larger chromatographic signal does not automatically indicate a higher absolute concentration.

GC-MS provides a useful means of comparing chemical fingerprints because compounds are separated chromatographically before their mass spectra are compared with reference spectra. Library matching is valuable for generating tentative assignments, but reliable structural identification generally requires

additional evidence, including authentic standards, retention-index agreement and appropriate spectral confirmation. GC-MS and related metabolomic approaches have been used to examine tomato volatile and semi-volatile constituents under different cultivars, maturity stages, storage conditions and processing treatments (Guan *et al.*, 2024; Zhang *et al.*, 2024; Zhang *et al.*, 2023; Xi *et al.*, 2021; Mellidou *et al.*, 2023; Leygeber *et al.*, 2022; Weinblum *et al.*, 2021; Yoo *et al.*, 2020). The present dataset contains one profile per condition, so the interpretation is deliberately descriptive rather than inferential.

The present work compares the GC-MS fingerprints of fresh tomato and tomato dried at 40, 50 and 60 °C. Specifically, the study sought to: (i) document the chromatographic information contained in the original instrument reports; (ii) examine the distribution of normalized peak areas across the four conditions; (iii) determine which tentative compound labels occurred across the profiles; and (iv) describe similarities and differences using summary statistics, Jaccard similarity and Bray-Curtis dissimilarity.

2. Materials and Methods

2.1 Sample and drying conditions

Fresh ripe tomato was used as the reference material, and the comparison included samples dried at 40, 50 and 60 °C. The purpose of the dataset was to characterize differences in the detectable chemical fingerprints associated with these drying conditions. It was not structured as a replicated quantitative experiment; accordingly, the results are presented as exploratory profile comparisons rather than statistical tests of treatment effects.

2.2 Extraction and GC-MS analysis

For extraction, 1 g of each tomato sample was treated with 5 mL of ethanol. The resulting extracts were analyzed on a Shimadzu GCMS-QP2010 Plus system. The instrument records indicated the use of a VF-5ms fused-silica capillary column (30 m × 0.25 mm × 0.25 µm) with an injection volume of 0.1 µL. Mass spectra were compared with the NIST05 library to generate tentative compound assignments. The reported peak areas were normalized so that each detected signal was expressed as a percentage of the total chromatographic response. Thus, the reported percentages describe relative signal contribution and should not be regarded as absolute concentrations.

2.3 Data processing

The original total-ion chromatogram reports were taken as the primary analytical records. Retention times and Area% values were transcribed directly from those reports. The fresh, 40, 50 and 60 °C chromatograms contained 13, 20, 25 and 26 reported peaks, respectively. Where the same library assignment appeared more than once across the profiles, the entries were consolidated by compound name, resulting in a comparison matrix containing 59 distinct tentative labels.

2.4 Descriptive and similarity analysis

For every original chromatographic profile, mean, median, standard deviation, minimum, maximum and coefficient of variation (CV) were obtained from the reported relative peak areas. Shannon diversity (H') was estimated from the normalized peak-area proportions using natural logarithms. Jaccard coefficients were calculated from the presence or absence of the 59 consolidated labels, while Bray-Curtis dissimilarity was calculated from the corresponding normalized peak-area matrix. Bray-Curtis similarity was then expressed as 1 - dissimilarity. These measures were used only to describe the observed fingerprints.

Inferential procedures such as ANOVA, t-tests, Tukey comparisons, p-values and significance groupings were not applied. Each temperature condition was represented by a single GC-MS profile, leaving no independent within-condition replicates from which experimental variance could be estimated. In the same way, a high relative peak area was not taken to mean that a compound was present at a higher absolute concentration, nor was its appearance interpreted as proof of formation during drying. Such claims would require replicated experiments, validated quantitative procedures and confirmation with authentic standards.

3. Results

3.1 Overall GC-MS profiles

The instrument records showed 13 chromatographic peaks in fresh tomato, compared with 20, 25 and 26 peaks in the samples dried at 40, 50 and 60 °C, respectively (Table 1). Within each profile, the normalized Area% values were approximately 100%, as expected from peak-area normalization. The number of reported chromatographic peaks should be understood as the number of observed signals and not as a direct count of unique chemical compounds.

Table 1. Number of reported chromatographic peaks and total normalized peak area for each tomato condition.

Sample	Detected peaks	Total normalized area (%)
Raw	13	99.99
40 °C	20	100.02
50 °C	25	99.99
60 °C	26	100.00

Note: The peak counts refer to chromatographic signals recorded by the instrument and should not be interpreted as counts of unique compounds.

3.2 Compounds represented across the four profiles

Combining repeated library assignments across the four datasets produced 59 distinct tentative compound labels. Only five labels ferulic acid, n-hexadecanoic acid, naringenin, “Quertine,” and lycopene had non-zero reported relative areas in fresh tomato as well as in all three dried conditions.

Table 2. Relative GC–MS signal contributions (%) for the five tentative labels present in all four profiles.

Compound	Fresh	40 °C	50 °C	60 °C
Ferulic acid	27.06	0.31	0.14	0.22
n-Hexadecanoic acid	25.73	8.97	4.73	1.81
Lycopene	0.82	0.35	9.43	0.41
Naringenin	1.90	1.01	0.70	0.32
Quertine	0.90	0.20	0.82	0.33

Note: The percentages are normalized GC-MS peak areas and therefore represent relative chromatographic contributions rather than absolute concentrations. Only labels with non-zero values in all four conditions are included.

Within this group of five labels, ferulic acid and n-hexadecanoic acid produced their largest relative signals in fresh tomato. Lycopene, in contrast, reached its highest normalized signal at 50 °C. The values for naringenin and the library label “Quertine” also differed among the drying conditions. These changes should be read as differences in chromatographic representation, not as direct measurements of concentration. Figure 1 summarizes the relative peak-area pattern for these five assignments.

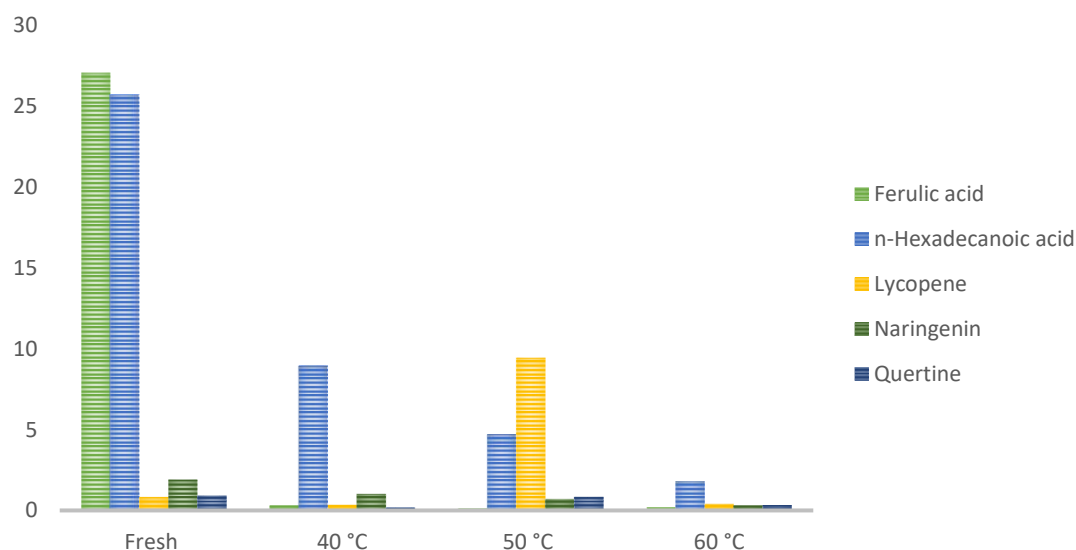


Figure 1. Comparison of normalized GC-MS peak-area contributions for five tentative assignments across fresh tomato and samples dried at 40, 50 and 60 °C.

Note: Values are relative peak-area percentages and indicate contributions to the chromatographic signal. Compound identities are tentative assignments obtained through library matching.

Table 3. Normalized GC–MS peak-area matrix for the 59 consolidated tentative compound labels.

Compound	Fresh	40 °C	50 °C	60 °C
Z-11-Hexadecenoic acid	0.00	59.95	0.00	0.00
Ethylene diacrylate	0.00	0.00	0.00	40.37
Erucic acid	0.00	0.00	32.90	0.00

Ferulic acid	27.06	0.31	0.14	0.22
n-Hexadecanoic acid	25.73	8.97	4.73	1.81
Oleic acid	21.90	0.00	0.00	0.00
9,12-Octadecadienoyl chloride	0.00	2.63	6.12	14.29
2-Methyl-Z,Z-3,13-octadecadienol	0.00	11.49	0.00	0.00
(Z)-7-Tetradecenal	0.00	0.00	11.04	0.00
Lycopene	0.82	0.35	9.43	0.41
4H-Cyclopentacycloocten-4-one, decahydro-	0.00	0.00	0.00	7.69
Octadecanoic acid	6.98	0.00	0.00	0.00
1,15-Hexadecadiene	0.00	0.00	6.31	0.00
13-Octadecenal, (Z)-	0.00	3.73	0.00	5.60
Hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester	0.00	0.00	0.00	5.46
Phenol, 3,5-bis(1,1-dimethylethyl)-	5.10	0.00	0.00	0.00
13-Octadecenoic acid, methyl ester	0.00	0.00	0.00	4.42
Hexadecanoic acid phospholipid ester	0.00	0.52	4.32	0.38
Hexadecanoic acid, 2,3-dihydroxypropyl ester	0.00	0.00	4.31	0.00
Dodecanoic acid, 4-methyl-, methyl ester	0.00	0.00	0.00	4.09
alpha-D-Galactopyranoside, methyl	0.00	0.00	3.59	0.00
9-Octadecenamide, (Z)-	0.00	1.17	3.28	0.00
Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester	0.00	0.00	0.00	3.09
3-Tetradecene, (Z)-	2.85	0.00	0.00	0.00
cis,cis-7,10-Hexadecadienal	0.00	0.00	2.60	0.00
Pentafluoropropionic acid, dodecyl ester	2.34	0.00	0.00	0.00
10-Octadecenoic acid, methyl ester	0.00	2.26	0.00	0.00
Pentadecanoic acid, 14-methyl-, methyl ester	0.00	0.00	0.49	2.18
Ethyl beta-D-ribose	0.00	0.00	2.10	0.00
9-Octadecenoic acid (Z)-, hexyl ester	0.00	0.00	2.09	0.00
9,12-Octadecadienoic acid, methyl ester	0.00	1.73	0.89	2.03
Carbamic acid, phenyl ester	2.02	0.00	0.00	0.00
Sucrose	0.00	0.00	1.99	0.00
2,3-Anhydro-D-galactosan	0.00	1.93	0.00	0.00
Naringenin	1.90	1.01	0.70	0.32

d-Gluco-heptulosan	0.00	0.00	0.00	1.74
1,3-Cyclopentadiene, 5-(1-methylethylidene)-	1.43	0.00	0.00	0.00
Cyclodecane	0.00	1.41	0.00	0.00
Octadecanoic acid, methyl ester	0.00	0.45	0.00	1.19
cis-11-Hexadecenal	0.00	0.00	0.00	1.17
Z,Z-4,16-Octadecadien-1-ol acetate	0.00	0.00	0.00	1.03
Benzene, (1-methylethyl)-	0.96	0.00	0.00	0.00
Quertine	0.90	0.20	0.82	0.33
Oxacycloheptadec-8-en-2-one	0.00	0.75	0.00	0.00
11-Octadecenoic acid, methyl ester	0.00	0.00	0.75	0.00
9,12-Tetradecadien-1-ol acetate	0.00	0.68	0.00	0.00
1-Octadecyne	0.00	0.00	0.00	0.64
Cyclopentane, 1-acetyl-1,2-epoxy-	0.00	0.00	0.63	0.00
Benzoylformic acid	0.00	0.00	0.00	0.43
Decanoic acid, 2-oxo-, methyl ester	0.00	0.00	0.00	0.42
Squalene	0.00	0.31	0.00	0.00
3,5-Dodecadiyne, 2-methyl-	0.00	0.00	0.00	0.31
1-Propanone, 1-(2-furanyl)-	0.00	0.00	0.26	0.00
1(2H)-Naphthalenone, 3,4,4a,5,8,8a-hexahydro-8a-methyl-, trans-	0.00	0.00	0.00	0.20
Hexadecanoic acid, 15-methyl-, methyl ester	0.00	0.00	0.20	0.00
2-Cyclopropylvinylidene-3-methoxy-1,1-dimethyl-cyclopropane	0.00	0.00	0.00	0.18
2-Oxepanone	0.00	0.00	0.18	0.00
2-Octanol, 8,8-dimethoxy-2,6-dimethyl-	0.00	0.17	0.00	0.00
Cyclopentane, butyl-	0.00	0.00	0.12	0.00

3.3 Major relative peak-area features

The fresh-tomato chromatogram was characterized by comparatively large signals assigned to ferulic acid (27.06%), n-hexadecanoic acid (25.73%), oleic acid (21.90%) and octadecanoic acid (6.98%). Additional signals of note included phenol, 3,5-bis(1,1-dimethylethyl)- (5.10%), (Z)-3-tetradecene (2.85%), pentafluoropropionic acid dodecyl ester (2.34%) and carbamic acid phenyl ester (2.02%). Together, these values describe the relative composition of the fresh reference profile.

At 40 °C, the largest normalized signal was assigned by the library to Z-11-hexadecenoic acid (59.95%). The next largest signals were 2-methyl-Z,Z-3,13-octadecadienol (11.49%) and n-hexadecanoic acid (8.97%), followed by (Z)-13-octadecenal (3.73%), 9,12-octadecadienoyl chloride (2.63%) and 10-octadecenoic acid methyl ester (2.26%).

The 50 °C profile was led by the tentative erucic acid assignment (32.90%). Other prominent signals included (Z)-7-tetradecenal (11.04%), lycopene (9.43%), 1,15-hexadecadiene (6.31%) and 9,12-octadecadienoyl chloride (6.12%).

At 60 °C, the highest relative signal was assigned to ethylene diacrylate (40.37%). This was followed by 9,12-octadecadienoyl chloride (14.29%), 4H-cyclopentacycloocten-4-one, decahydro- (7.69%), (Z)-13-octadecenal (5.60%), hexadecanoic acid, 2-hydroxy-1,3-propanediyl ester (5.46%) and 13-octadecenoic acid, methyl ester (4.42%).

The dominant signals should be treated as characteristics of the recorded chromatograms rather than as chemically confirmed constituents. Because normalization forces the peak areas within each profile to a common total, the percentage assigned to one component is influenced by the relative contribution of the remaining components. In addition, library matching alone does not establish compound identity with certainty. This is especially important for assignments that appear chemically unusual in a tomato matrix; those entries require independent confirmation before they can be discussed as genuine constituents or drying products.

3.4 Descriptive statistics

The descriptive measures calculated from the original peak-area records are summarized in Table 4. The mean relative peak area decreased from 7.69% in the fresh profile to 3.85% at 60 °C. Median values ranged from 1.09% at 40 °C to 2.34% in fresh tomato. The Shannon index was lowest at 40 °C (1.582) and highest at 50 °C (2.426), indicating differences in how the normalized chromatographic signal was distributed among the detected peaks. These figures are descriptive and do not provide a statistical test of drying-temperature effects.

Table 4. Descriptive statistics calculated from the four original GC–MS profiles.

Condition	peaks	Mean area (%)	Median (%)	SD	Minimum (%)	Maximum (%)	CV (%)	Shannon H'
Fresh	13	7.69	2.34	10.02	0.82	27.06	130.30	1.904
40 °C	20	5.00	1.09	13.27	0.17	59.95	265.32	1.582
50 °C	25	4.00	2.09	6.70	0.12	32.90	167.46	2.426
60 °C	26	3.85	1.18	8.09	0.18	40.37	210.33	2.210

3.5 Jaccard similarity of detection profiles

The Jaccard coefficients fell between 0.15 and 0.28 (Table 5), showing that only a relatively small proportion of the consolidated tentative labels was shared between the different conditions. The greatest label overlap occurred between the 40 and 60 °C profiles (0.28), followed by the 40 and 50 °C profiles (0.25). Fresh tomato compared with either 50 or 60 °C gave the lowest coefficient (0.15). These coefficients describe shared detection patterns and are not significance tests.

Table 5. Pairwise Jaccard similarity coefficients for the four tomato GC–MS detection profiles.

Sample	Fresh	40 °C	50 °C	60 °C
Fresh	1.00	0.18	0.15	0.15
40 °C	0.18	1.00	0.25	0.28
50 °C	0.15	0.25	1.00	0.21
60 °C	0.15	0.28	0.21	1.00

Note: Jaccard similarity is based on presence or absence of the 59 consolidated tentative labels. The values are descriptive and were not subjected to inferential significance testing.

3.6 Bray-Curtis similarity and dissimilarity

Across the treatment pairs, Bray-Curtis dissimilarity ranged from 0.882 to 0.969, corresponding to similarities from 0.118 to 0.031 (Table 6). The 40 and 60 °C profiles had the smallest dissimilarity (0.882) and consequently the greatest abundance-weighted similarity (0.118). The fresh and 60 °C profiles were the most separated, with a dissimilarity of 0.969 and a similarity of 0.031. Unlike Jaccard analysis, which considers only whether a label occurs, Bray-Curtis also incorporates the relative magnitude of the signals.

Table 6. Pairwise Bray–Curtis dissimilarity and similarity for the four tomato GC–MS profiles.

Sample	Fresh	40 °C	50 °C	60 °C
Fresh	0.000/1.000	0.892/0.108	0.928/0.072	0.969/0.031
40 °C	0.892/0.108	0.000/1.000	0.887/0.113	0.882/0.118

50 °C	0.928/0.072	0.887/0.113	0.000/1.000	0.891/0.109
60 °C	0.969/0.031	0.882/0.118	0.891/0.109	0.000/1.000

Note: Each entry gives dissimilarity/similarity. Dissimilarity ranges from 0 for identical profiles to 1 for maximum separation; similarity was calculated as 1 - dissimilarity. The analysis used the 59-compound relative peak-area matrix and is descriptive.

3.7 Original chromatographic profiles

The total-ion chromatograms in Figure 2 visually demonstrate that the four conditions produced different signal patterns. Fresh tomato had fewer reported peaks, whereas the dried samples displayed additional signals and distinct high-intensity regions. The chromatograms therefore support the observation that the detectable GC-MS fingerprints changed with drying condition. They do not, by themselves, establish the identity or absolute quantity of the compounds associated with individual peaks.

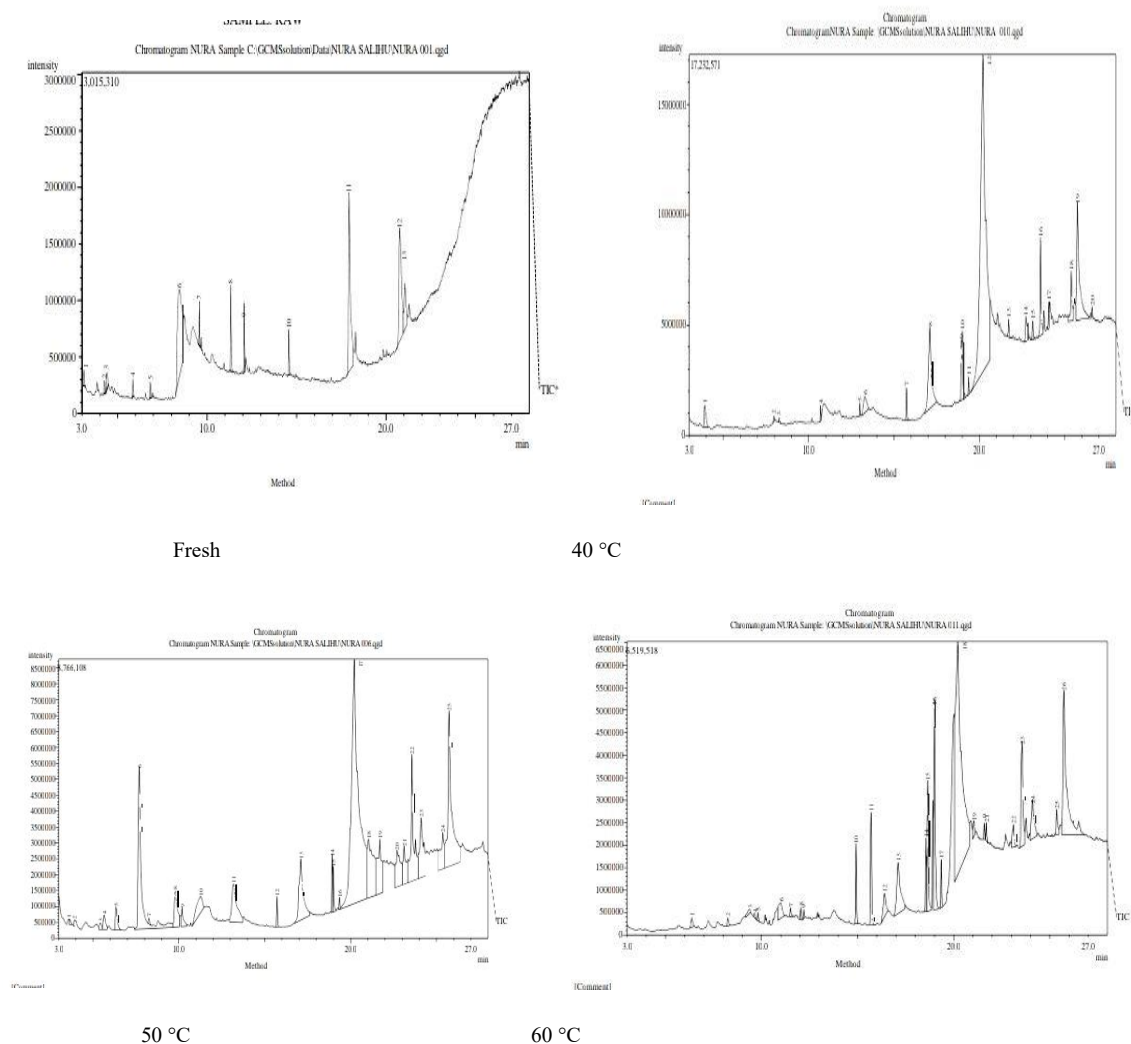


Figure 2. Original GC-MS total-ion chromatograms recorded for fresh tomato and tomato dried at 40, 50 and 60 °C.

4. Discussion

4.1 Overall effect of drying on the GC-MS fingerprint

A clear change in the overall GC-MS fingerprint accompanied the drying treatments. The instrument reports contained 13 peaks in fresh tomato and 20, 25 and 26 peaks after drying at 40, 50 and 60 °C, respectively. Similar changes in food chemical profiles have been associated with dehydration because moisture loss, thermal exposure, structural modification of the matrix and changes in extraction behaviour can alter the compounds observed analytically (Al Maiman *et al.*, 2021; Degwale *et al.*, 2022; Pravitha *et al.*, 2024; Alemayehu *et al.*, 2026). Temperature-dependent responses have also been reported for tomato quality and bioactive constituents during drying (Mwende *et al.*, 2018; Obadina *et al.*, 2018; Tan *et al.*, 2021; Dufera *et al.*, 2021; Correia *et al.*, 2015; Cruz *et al.*, 2012; Bakir *et al.*, 2023).

The increase in a library-assigned signal after drying should not automatically be interpreted as chemical synthesis. Several processes can produce an altered chromatographic pattern. Removal of water can increase the relative representation of non-water components, while heat-induced changes in tissue structure may release compounds that were less accessible in the fresh matrix. At the same time, susceptible constituents may decline because of oxidation, degradation or other thermal reactions. These possibilities have been discussed in studies of dried horticultural materials and tomato products (ElGamal *et al.*, 2023; Nzimande *et al.*, 2025; Li *et al.*, 2022; Hossain *et al.*, 2024; Farid *et al.*, 2022). Changes in antioxidant properties with drying temperature have likewise been reported for tomato powder (Kim & Chin, 2016). The present single-profile dataset cannot distinguish among these mechanisms.

4.2 Fresh tomato profile

In the fresh sample, the most prominent relative signals were assigned to ferulic acid, n-hexadecanoic acid, oleic acid and octadecanoic acid. These signals provide the baseline against which the dried profiles can be compared. Tomato is known to contain phenolic acids, flavonoids, carotenoids and lipid-related constituents, but the amount detected by GC-MS depends on the extraction procedure, chromatographic conditions, ionization behaviour and reliability of spectral-library matching (Ali *et al.*, 2021; Lima *et al.*, 2022; Manzo *et al.*, 2018; Felföldi *et al.*, 2021).

The large normalized signals observed for ferulic acid and the fatty-acid-related assignments should be understood as percentages of the chromatographic response, not percentages of the tomato itself. Peak-area normalization produces compositional data: when the relative contribution of one signal changes, the percentages of other signals can change even if their absolute quantities do not change in the same proportion. This limitation is particularly important when comparing fresh and dried matrices.

4.3 Profile at 40 °C

The 40 °C chromatogram was dominated by the tentative Z-11-hexadecenoic acid assignment, which represented 59.95% of the normalized signal. It was followed by 2-methyl-Z,Z-3,13-octadecadienol (11.49%) and n-hexadecanoic acid (8.97%). The marked difference from the fresh profile shows that the detectable fingerprint under the mild drying condition was different. Moisture loss, changes in matrix structure and differences in extraction recovery could all contribute to this observation. However, the available data cannot determine which mechanism predominated, and the result does not prove that the assigned compound was generated during drying.

4.4 Profile at 50 °C

A different pattern was obtained at 50 °C. Erucic acid was the largest tentative assignment (32.90%), followed by (Z)-7-tetradecenal (11.04%), lycopene (9.43%), 1,15-hexadecadiene (6.31%) and 9,12-octadecadienoyl chloride (6.12%). Among the four conditions, the lycopene signal was greatest at this temperature. Previous research indicates that tomato carotenoids may respond differently to processing depending on temperature and matrix conditions, with changes arising from both thermal losses and altered accessibility or extractability (Ali *et al.*, 2021; Wu *et al.*, 2022; Nzimande *et al.*, 2025; Li *et al.*, 2022).

The lycopene result should therefore be described specifically as the highest relative GC-MS signal observed at 50 °C. It should not be presented as evidence that the absolute lycopene concentration increased during drying. Demonstrating a true concentration change would require calibration against an authentic lycopene standard or another validated quantitative analytical procedure.

4.5 Profile at 60 °C

At 60 °C, ethylene diacrylate produced the largest library-assigned peak (40.37%), followed by 9,12-octadecadienoyl chloride (14.29%), 4H-cyclopentacycloocten-4-one, decahydro- (7.69%), (Z)-13-octadecenal (5.60%), and other oxygenated or lipid-associated assignments. The prominence of these signals indicates that the 60 °C chromatographic fingerprint differed markedly from both fresh tomato and the lower-temperature dried samples.

4.6 Lycopene and phenolic-related signals

Lycopene occurred in all four chromatographic profiles, but its normalized signal reached the maximum value at 50 °C (9.43%). This observation is consistent with the broader importance of tomato carotenoids and with reports showing that processing can influence carotenoid retention, release and extractability (Ali *et al.*, 2021; Wu *et al.*, 2022; Nzimande *et al.*, 2025; Li *et al.*, 2022). Ferulic acid showed a contrasting pattern, with its largest normalized contribution occurring in the fresh sample. Neither pattern should be interpreted as a direct measure of absolute concentration because the data are based on within-profile normalization.

4.7 Similarity among the four profiles

The Jaccard results show relatively limited sharing of the consolidated tentative labels among the four conditions. The 40 and 60 °C profiles had the highest coefficient (0.28), whereas the comparisons of fresh tomato with 50 °C and 60 °C produced the lowest value (0.15). The pattern agrees with the visible differences in the chromatograms and with the use of metabolomic and volatilomic approaches to examine condition-dependent changes in tomato chemistry (Guan *et al.*, 2024; Zhang *et al.*, 2024; Xi *et al.*, 2021; Mellidou *et al.*, 2023; Leygeber *et al.*, 2022; Weinblum *et al.*, 2021). The low overlap indicates that the detectable fingerprint changed considerably across the processing conditions, although the analysis cannot establish the biochemical mechanism responsible.

4.8 Bray-Curtis comparison of abundance-weighted profiles

Bray-Curtis analysis adds information about the magnitude of the normalized signals to the presence/absence information provided by Jaccard similarity. The 40 and 60 °C samples showed the greatest abundance-weighted similarity (0.118) and the smallest dissimilarity (0.882). In contrast, fresh tomato versus 60 °C produced the largest dissimilarity (0.969) and the lowest similarity (0.031). Thus, the two similarity measures provide complementary descriptions: Jaccard reflects shared labels, whereas Bray-Curtis also considers how strongly those labels contribute to the chromatographic profile.

4.9 Statistical interpretation and limitations

The Shannon index provides another way of describing the distribution of normalized peak areas within each profile. Its highest value was observed at 50 °C (2.426), while the lowest was recorded at 40 °C (1.582). These values indicate differences in the distribution of chromatographic signal among detected peaks, but they should not be treated as evidence of a statistically significant temperature effect. With only one profile per condition, the reproducibility of these diversity patterns cannot be evaluated.

The most important limitation is the absence of independent biological or analytical replicates. Without replication, within-condition variability cannot be estimated and inferential procedures such as ANOVA cannot be appropriately supported. A further limitation is that compound identities were inferred from spectral-library matching rather than confirmed with authentic standards. This is particularly relevant for assignments that are chemically unexpected in tomato. Confirmation should include authentic standards, retention-index comparison, examination of diagnostic mass-spectral ions and, where appropriate, complementary analytical techniques. The study should therefore be regarded as an exploratory GC-MS fingerprinting exercise that generates candidates for subsequent quantitative and structural validation.

5. Conclusion

The GC-MS profiles differed noticeably between fresh tomato and the samples dried at 40, 50 and 60 °C. The original instrument records contained 13, 20, 25 and 26 chromatographic peaks, respectively, and consolidation of the reported library assignments resulted in 59 distinct tentative labels. Fresh tomato was characterized by relatively large signals assigned to ferulic acid and several fatty-acid-related compounds, whereas each dried condition displayed its own dominant signals. The lycopene-associated signal reached its highest relative value at 50 °C. Jaccard analysis showed limited overlap among the four detection profiles, while Bray-Curtis analysis indicated substantial differences in the abundance-weighted distribution of the normalized signals.

These findings should be interpreted within the limits of the analytical design. One GC-MS profile was available for each condition, and the compound names were obtained through tentative spectral-library matching. Consequently, the dataset can demonstrate differences in the observed fingerprints but cannot establish absolute concentration changes, statistically significant treatment effects or confirmed thermal formation of individual compounds. The results are most appropriately considered hypothesis-generating. Future studies should include biological and analytical replication, authentic reference standards, retention-index verification and validated quantitative methods to determine whether the observed profile differences correspond to genuine changes in compound concentration or identity.

Declarations

Data availability: The comparative GC-MS dataset was obtained from the original instrument reports used for this study. The complete instrument records and chromatograms should be preserved as the primary analytical evidence and shared when permitted by the laboratory and the journal.

Conflict of interest: The authors report no conflict of interest associated with this study.

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