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Studies on Volatile Aromatic Compounds Associated with Spoilt Tomatoes in Sokoto Metropolis, Sokoto State, Nigeria

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This study used GC-MS to analyze the VOC profiles of spoiled tomatoes, identifying potential spoilage markers. Spoiled tomatoes exhibited distinct VOC signatures, including aldehydes, alcohols, esters, hydrocarbons, and fatty acids, which were minimal or absent in fresh tomatoes. These VOCs likely originated from lipid breakdown, microbial involvement, and enzymatic fat breakdown. Quantifying these VOCs could lead to non-invasive methods for monitoring tomato quality, reducing food spoilage and waste. Specific VOCs, such as aldehydes (e.g., butanal-3-hydroxy, pentanal), likely originated from lipid breakdown products and potentially contributed to off-odors. Alcohols (e.g., 2-hexanol, 4-methyl-2-hexanol) might indicate microbial involvement, while the presence of esters (e.g., methoxyacetic acid octyl ester) suggested potential consequences of advanced spoilage. Fatty acids and their derivatives (e.g., methyl esters, oleic acid) pointed towards enzymatic breakdown of fats during spoilage. Epoxides (e.g., cis-2,3-dimethyloxirane) were detected in some spoiled samples, warranting further investigation.

Keywords: Volatile organic compounds (VOCs), spoilage markers, microbial activity, fatty acids, tomato and food quality.

1. Introduction

Tomatoes (*Lycopersicon esculentum*) are a widely consumed vegetable in Nigeria and globally, rich in nutrients like carbohydrates, fats, organic acids, water, minerals, vitamins, and pigments. However, their high water content makes them susceptible to spoilage by microorganisms, leading to reduced nutritional and market value (Maddox, 2008; FAO, 2020). Volatile organic compounds (VOCs) play a crucial role in tomato flavor and aroma, with over 400 identified volatiles contributing to their characteristic taste and smell (Yilmaz, 2001; Aprea *et al.,* 2020). VOCs also serve as indicators of tomato quality and spoilage, making their detection essential for monitoring tomato freshness and safety (Berna *et al.,* 2019). This research aims to identify the microorganisms associated with tomato spoilage and the VOCs emitted by spoilt tomatoes, providing valuable insights for improving tomato storage, transportation, and quality control.

Tomato spoilage is a significant problem in the food industry, resulting in economic losses and reduced food quality. The current methods for detecting spoilage are limited, and there is a need for a non-invasive and rapid method for monitoring tomato quality. The use of GC-MS analysis will provide a comprehensive understanding of the VOC profiles of spoiled tomatoes, which can lead to the development of non-invasive methods for monitoring tomato quality. The findings of this study will contribute to the existing knowledge on tomato spoilage and VOC analysis, and they will have practical applications in the food industry.

Tomato (*Lycopersicon esculentum*) is a widely cultivated crop globally, but its fruit is susceptible to spoilage, particularly due to fungal infections (Ghosh, 2009). Wilts caused by *Fusarium* oxysporum and *Pseudomonas solanacearum* are significant diseases affecting tomato crops in Nigeria and other countries (Erinle, 2006; El-Abyad *et al.,* 1993; El-Shanshoury *et al.,* 1996; Qasem, 2006; Sharma and Norwak, 2008; De Cal *et al.,* 2009). Recent studies have focused on identifying the volatile organic compounds (VOCs) associated with spoiled tomatoes. Ghosh (2009) found that fungi, particularly *Aspergillus niger* and Fusarium, were the primary causes of spoilage in tomato samples, with a few samples containing Penicillium sp. Similarly, a study by Zhang *et al.* (2020) detected Fusarium and Aspergillus species in spoiled tomatoes, with

VOCs analysis revealing the presence of compounds like hexanal, 2-hexenal, and 3-octanone.In contrast, a study by Bhattacharya *et al.* (2018) identified bacterial spoilage in tomatoes, with VOCs analysis detecting compounds like trimethylamine, dimethyl sulfide, and acetic acid. However, their methodology differed from Ghosh (2009) and Zhang *et al.* (2020), as they used a different sampling method and VOCs analysis technique. A recent review by Aprea *et al.* (2020) highlighted the importance of VOCs in monitoring tomato quality and spoilage. They noted that VOCs can be used as biomarkers for early detection of spoilage, but the variability in VOC profiles among different tomato varieties and spoilage microorganisms requires further research. Overall, while there is consensus on the role of fungi in tomato spoilage, the variability in VOC profiles and the need for standardized methodologies for VOCs analysis are areas that require further investigation. This study was undertaken to investigate the volatile aroma compounds associated with spoilt tomatoes.

2. Materials and Methods

2.1 Materials

Ten samples of spoilt tomatoes and One (1) sample of healthy, freshly harvested tomatoes, sterile distilled water, sterile test tubes, mortar and pestle, blender, Petri dishes containing solidified medium, Lactophenol Cotton Blue Mount (LPCB) stain, microscope slides, distilled water (for microscopy), cover slips, glass slides (for Gram staining), crystal violet stain, Lugol's solution, safranin stain, chemicals and reagents for specific biochemical tests (not specified), Lenton furnaces, Gallenkamp Oven BS, Soxhlet extraction apparatus, chloroform/methanol solvent (2:1 mixture), n-Hexane, Kjeldahl digestion apparatus (for Micro-kjeldahl Method), bottles, diethyl ether, Whatman No. 1 filter paper, GCMS-QP2010 plus (Shimadzu, Japan) equipped with a flame ionization detector (FID), DB-WAX analytical column (30 m 0.25 mm, 0.25mm, J&W scientific, Folsom C.A), helium gas.

2.2 Methods

2.2.1 Sample Collection

A total of ten samples (10) of spoilt tomatoes and 1 (one) sample of healthy freshly harvested tomatoes were collected from five (5) various sources namely; Kasuwan-Daji, Guiwa low-cost, Bado Area, Polo Club and Sokoto Central Market. The samples were obtained from local sellers (those that have change in color, with bruises, and mold as well as soft in texture were regarded as spoilt, on the hand fresh tomato looks red without discoloration and it's hard in texture, The samples were collected aseptically in clean labeled containers and transported to the Microbiology laboratory of Sokoto State University for analyses.

2.2.2 Extraction of volatile Metabolites

Volatile compounds were extracted using a direct solvent extraction method as described by Ibrahim *et al.* (2011). The extraction of volatile compounds followed a direct solvent extraction method. Two grams of spoilt tomatoes and healthy ripe tomatoes were weighed into a bottle and saturated with 20ml of diethyl ether. The mixture was allowed to stand at 28°C for 24 hours. The extract was then filtered using Whatman No. 1 filter paper, and the filtrate was collected in a sterile bottle, closed tightly before the GC-MS analysis.

2.2.3 Gas Chromatography Mass Spectrometry (GC-MS) Analysis

GC-MS analysis was performed using a GCMS-QP2010 plus (Shimadzu, Japan) equipped with a flame ionization detector (FID). The injection was conducted in splitless mode at 250°C for 3 minutes using an inlet of 0.75mm i.d. to minimize peak broadening. Chromatographic separations were performed using a DB-WAX analytical column 30 m 0.25 mm, 0.25mm (J&W scientific, Folsom C.A) with helium as the carrier gas at a constant flow rate of 0.8 ml/Min. The oven temperature was programmed at 60°C for 5 minutes, followed by an increase (held for 5 minutes), and finally at 10°C/min to 280°C (held for 10 minutes). The temperature of the FID was set to 250°C. MS operating conditions used electron impact ionization mode with an ion source temperature of 200°C, ionization voltage of 70 eV, and a mass scan range of m/z 23-450 at 2.76 scans/s.

The identification of chromatographic peak was carried out by comparing their mass spectra with those of the bibliography data of known compounds from the NIST library mass spectra database on the basis of the criterion similarity (SI)>800 (the highest value being 1,000). According to the method of [13] approximate quantification of volatile compounds was estimated by the integration of peaks on the total ion chromatogram using Xcalibur software (Vienna, VA). The results are presented as the peak area normalized (%).

3. Results and Discussion

3.1 Results

The results of the GC –MS analyses for fresh tomatoes are presented in Tables 1 – 10; while that of the spoiled tomatoes is as presented in Table 11.

Table 1: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 1)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
	7.068	22.2258	Butanal, 3-hydroxy-	2056	000107-89-1	35
2	7.1147	7.3969	1H-Pyrrole, 2,5-dihydro-1-nitroso-	3088	010552-94-0	43
3	7.2229	6.8372	Benzaldehyde, 3,5-dichloro-2-hydroxy-, 2,2-dimethylhydrazone	95309	014490-83-6	38
4	7.35	6.9583	8,9,9,10,10,11-Hexafluoro-4,4-dimethyl-3,5-dioxatetracyclo[5.4.1.0(2,6).0(8,11)]dodecane	160960	1000223-08-6	32
5	12.07	-4.3291	1H-Pyrrole, 2,5-dihydro-1-nitroso-	3088	010552-94-0	50
6	12.2513	1.0887	Butanal, 3-hydroxy-	2056	000107-89-1	46
7	12.3369	0.2893	Pentanal	1727	000110-62-3	43
8	12.3904	0.1586	1H-Isoindole, 2,3,3a,4,7,7a-hexahydro-	10425	1000351-26-7	38
9	16.6714	-5.9622	4-Fluorohistamine	13121	049872-60-8	64
10	16.7022	0.0544	Butanal, 3-hydroxy-	2056	000107-89-1	58
11	16.7306	0.0628	Propane, 2-(ethenyloxy)-	1815	000926-65-8	55
12	16.7684	0.0968	Butanal, 3-hydroxy-	2056	000107-89-1	58
13	16.8108	0.0191	Pterin-6-carboxylic acid	71717	000948-60-7	53
14	22.2812	1.1093	Butanal, 3-hydroxy-	2056	000107-89-1	46
15	22.3294	0.1633	Butanal, 3-hydroxy-	2056	000107-89-1	38
16	22.3546	0.1703	Butanal, 3-hydroxy-	2056	000107-89-1	43
17	27.221	3.5838	Hexadecanoic acid, methyl ester	130813	000112-39-0	98
18	28.8941	15.9947	9,12-Octadecadienoic acid, methyl ester	153873	002462-85-3	99
19	28.9721	40.0285	trans-13-Octadecenoic acid, methyl ester	155762	1000333-61-3	99
20	29.2437	0.7107	Methyl stearate	157879	000112-61-8	99
21	35.3293	0.5199	Cyclononasiloxane, octadecamethyl-	274624	000556-71-8	86
22	36.2783	0.5946	1,1,1,5,7,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetrasiloxane	254928	038147-00-1	53
23	37.0132	0.465	Hentriacontane	252711	000630-04-6	89
24	37.3636	2.0242	N-Benzyl-N-ethyl-p-isopropylbenzamide	141055	015089-22-2	38
25	45.5501	-0.5475	7,11-Hexadecadienal	98680	1000130-85-7	93
26	45.9299	0.2867	Butanamide, 3-cyclohexylamino-4-hydroxy-N-cyclohexyl-	141872	1000260-52-8	22

Table 2: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 2)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	19.4688	0.289	trans-1-Chloromethyl-2-methoxymethylcyclohexane	45024	137303-15-2	38
2	19.5078	0.2546	2-Hydroxy-3-pentanone	4331	005704-20-1	47
3	19.6416	0.0573	Methoxyacetic acid, octyl ester	66467	029267-10-5	50
4	19.7072	0.0338	2-Formylhistamine	18162	1000132-95-8	47
5	19.7423	0.0189	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	38
6	19.8086	0.0134	2-Hexanol	4480	000626-93-7	47
7	19.8786	0.031	Phenelzine	16567	000051-71-8	43
8	19.9175	0.0168	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	53
9	20.1107	0.1039	1-Butaneboronic acid	4291	004426-47-5	53
10	20.1561	0.0381	2-Hexanol, 3-methyl-	8497	002313-65-7	53
11	20.2863	5.3125	2,5-cyclohexadien-1-one, 2,6-bis(1,1-dimethylethyl)-4-hydroxy-4-methyl-	98565	1000401-12-0	64
12	20.4498	0.3884	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	59

13	20.4721	0.7477	Pentane, 1-methoxy-	4507	000628-80-8	38
14	20.5323	0.2001	3-Nitropropanoic acid	9175	000504-88-1	47
15	20.5559	0.4105	(3-Oxo-3H-benzo[f]chromen-1-yl)-acetic acid ethyl ester	141913	1000296-72-0	53
16	20.5915	0.1831	Butanal, 3-hydroxy-	2055	000107-89-1	64
17	20.6159	0.2171	m-Dioxan-4-ol, 2,6-dimethyl-	14608	004740-77-6	53
18	20.7225	1.0303	Phenelzine	16566	000051-71-8	43
19	20.748	1.1771	4-Methyl-2-hexanol	8491	002313-61-3	47
20	20.982	9.9572	ButylatedHydroxytoluene	83558	000128-37-0	98
21	27.4259	0.3611	Dibutyl phthalate	138058	000084-74-2	78
22	28.1053	0.257	n-Hexadecanoic acid	117416	000057-10-3	58
23	28.1724	1.2425	n-Hexadecanoic acid	117419	000057-10-3	99
24	29.5346	0.4323	Z,Z-6,13-Octadecadien-1-ol acetate	167383	1000131-07-0	86
25	29.8546	0.1609	Z,Z-10,12-Hexadecadien-1-ol acetate	140149	1000130-89-5	74
26	29.9423	0.1592	2-Methyl-Z,Z-3,13-octadecadienol	140253	1000130-90-5	78
27	30.018	0.1334	Cyclotetradecane	61850	000295-17-0	87
28	30.9064	0.259	Tricosane	182655	000638-67-5	89
29	31.7561	0.1992	Decane, 2-methyl-	29360	006975-98-0	64
30	32.569	0.2624	Hentriacontane	252712	000630-04-6	87
31	32.7121	0.6165	Di-n-octyl phthalate	233363	000117-84-0	91
32	33.3605	0.2976	Tritetracontane	273205	007098-21-7	76
33	34.1189	0.339	Cycloeicosane	140274	000296-56-0	92
34	34.8496	0.5817	Eicosane	142240	000112-95-8	89
35	34.9131	1.7298	Supraene	243217	007683-64-9	96
36	35.0581	0.3341	Oleic Acid	142070	000112-80-1	59
37	35.1687	0.5649	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	60
38	35.5533	8.9366	Heptadecane, 9-hexyl-	182660	055124-79-3	93
39	35.6846	0.7585	9,12-Octadecadien-1-ol, (Z,Z)-	126846	000506-43-4	91
40	36.241	27.1677	1-Octadecanesulphonyl chloride	206960	1000342-70-4	55
41	36.3807	1.8668	9-Octadecenoic acid	142074	002027-47-6	56
42	36.4157	1.1856	2-Methylaminomethyl-1,3-dioxolane	8669	057366-77-5	22
43	36.4589	2.2556	9,12-Octadecadienoyl chloride, (Z,Z)-	157778	007459-33-8	92
44	36.4786	2.0584	6-Nitroundec-5-ene	64169	1000192-40-3	44
45	36.5231	1.52	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	50
46	36.5478	1.4284	Butyl 9-octadecenoate or 9-18:1	195600	1000336-74-7	45
47	36.6014	4.0208	7,11-Hexadecadienal	98680	1000130-85-7	44
48	36.656	2.0408	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	42
49	36.7088	5.7755	Oleic Acid	142070	000112-80-1	52
50	37.0069	9.4047	Hexacosane	217892	000630-01-3	97
51	39.4742	0.3605	Caparratriene	70754	1000374-08-7	48
52	43.0489	-0.0188	Oleic Acid	142070	000112-80-1	46
53	43.168	0.0485	Cyclopenta[c]furo[3',2':4,5]furo[2,3-h][1]benzopyran-11(1H)-one, 2,3,6a,9a-tetrahydro-1,3-dihydroxy-4-methoxy-	187901	055446-27-0	42
54	43.4033	0.0341	3-Octyne, 6-methyl-	10827	062108-34-3	20
55	43.4671	0.0229	9-Oxabicyclo[6.1.0]nonane	11611	000286-62-4	90
56	43.536	0.0474	7,11-Hexadecadienal	98680	1000130-85-7	62
57	43.6924	0.2448	9-Oxabicyclo[6.1.0]nonane	11611	000286-62-4	90
58	43.8074	0.4248	3-Octyne, 6-methyl-	10827	062108-34-3	30
59	43.8746	0.4912	9,12-Octadecadien-1-ol, (Z,Z)-	126846	000506-43-4	50

60	43.9366	0.3207	7,11-Hexadecadienal	98680	1000130-85-7	50
61	43.9679	0.2364	Cyclopentadecanone, 2-hydroxy-	102369	004727-18-8	90
62	43.9958	0.2191	Hexadecenoic acid, Z-11-	115324	002416-20-8	44
63	44.0356	0.2625	Oleic Acid	142070	000112-80-1	50
64	44.0612	0.1257	9-Oxabicyclo[6.1.0]nonane	11611	000286-62-4	91
65	44.0829	0.1323	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	47
66	44.1083	0.0843	9-Oxabicyclo[6.1.0]nonane	11611	000286-62-4	48
67	44.1321	0.0595	7,11-Hexadecadienal	98680	1000130-85-7	56
68	44.1548	0.0734	Oleic Acid	142070	000112-80-1	20

Table 3: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 3)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	27.2413	2.0864	Hexadecanoic acid, methyl ester	130818	000112-39-0	97
2	27.423	0.3432	Didodecyl phthalate	266710	002432-90-8	52
3	28.6143	0.1588	Oxirane, 2,3-dimethyl-, cis-	711	001758-33-4	46
4	28.8824	5.8384	9,12-Octadecadienoic acid, methyl ester	153873	002462-85-3	99
5	28.9528	6.5904	10-Octadecenoic acid, methyl ester	155731	013481-95-3	98
6	29.2514	0.3542	Methyl stearate	157880	000112-61-8	96
7	37.011	0.38	Tricosane	182655	000638-67-5	95
8	39.5018	3.5078	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	210562	000111-03-5	44
9	39.5527	0.5018	Oleic Acid	142070	000112-80-1	50
10	39.61	1.3256	Oleic Acid	142070	000112-80-1	51
11	39.6848	1.5222	Oleic Acid	142070	000112-80-1	25
12	39.7306	1.0464	9-Oxabicyclo[6.1.0]nonane	11611	000286-62-4	62
13	39.7573	0.8198	9,12-Octadecadienoyl chloride, (Z,Z)-	157778	007459-33-8	92
14	39.9541	6.0209	9-Oxabicyclo[6.1.0]nonane, cis-	11674	004925-71-7	48
15	40.2644	15.865	Oleic Acid	142070	000112-80-1	38
16	40.3164	3.6264	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	72
17	40.3664	3.3738	9-Oxabicyclo[6.1.0]nonane	11611	000286-62-4	66
18	40.4609	6.9019	Z-6-Pentadecen-1-ol acetate	128651	068760-72-5	47
19	40.4839	11.8515	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	58
20	40.6529	27.8857	9-Oxabicyclo[6.1.0]nonane, cis-	11674	004925-71-7	55

Table 4: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 4)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	7.4072	0.9725	Propanamide, N-acetyl-	7888	019264-34-7	35
2	8.3893	0.8734	Hydroperoxide, 1-methylbutyl	4872	014018-58-7	38
3	12.4381	38.5918	Propanamide, N-acetyl-	7888	019264-34-7	38
4	18.9745	2.1344	N,N-Dimethylethanesulfonamide	16970	006338-68-7	43
5	19.5181	1.3663	Ethanone, 1-(2-benzothiazolyl)-	45629	001629-78-3	10
6	19.6496	0.2417	.alpha.-Acetyl-N,N-dinormethadol	183312	040488-01-5	25
7	20.2801	3.57	2,5-cyclohexadien-1-one, 2,6-bis(1,1-dimethylethyl)-4-hydroxy-4-methyl-	98565	1000401-12-0	90
8	20.9914	3.6892	ButylatedHydroxytoluene	83554	000128-37-0	98
9	22.1051	8.7291	Oxirane, 2,3-dimethyl-, cis-	711	001758-33-4	47
10	22.1687	0.5757	Octanal	12693	000124-13-0	37
11	22.232	0.7637	.alpha.-l-Mannose semicarbazonepentaacetate	262385	1000130-10-0	32
12	22.2883	0.6663	Oxirane, 2,3-dimethyl-, cis-	711	001758-33-4	50
13	22.4201	9.3857	Butanedioic acid, 2,3-bis(acetyloxy)-, [R-(R*,R*)]-	96985	051591-38-9	47
14	35.5532	0.0579	Carbonic acid, eicosyl vinyl ester	219345	1000382-54-3	70

15	36.2676	0.065	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	266854	019095-23-9	32
16	37.0131	0.1635	Eicosane	142240	000112-95-8	96
17	38.7077	0.2121	9,17-Octadecadienal, (Z)-	125003	056554-35-9	83
18	39.0051	0.0977	7-Hexadecenal, (Z)-	100566	056797-40-1	42
19	39.4776	0.2919	2-Methyl-Z,Z-3,13-octadecadienol	140253	1000130-90-5	46
20	39.805	0.0966	9-Oxabicyclo[6.1.0]nonane, cis-	11674	004925-71-7	86
21	40.4991	0.6264	6-Octadecenoic acid, (Z)-	142084	000593-39-5	45
22	43.1205	26.829	7,11-Hexadecadienal	98680	1000130-85-7	89

Table 5: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 5)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	7.7433	22.4134	1-Butanol	841	000071-36-3	53
2	13.4922	0.0644	Oxirane, 2-butyl-3-methyl-, cis-	7744	056052-93-8	53
3	17.2134	0.0326	1,2-Hydrazinedicarboxylic acid, diethyl ester	44694	004114-28-7	43
4	18.6218	0.2527	Diethyl carbonate	8847	000105-58-8	53
5	20.2955	3.6083	Hydrazinecarboxylic acid, ethyl ester	4726	004114-31-2	38
6	20.9956	7.588	ButylatedHydroxytoluene	83558	000128-37-0	95
7	21.2389	5.0613	Oxirane, 2-butyl-3-methyl-, cis-	7744	056052-93-8	52
8	21.5637	3.7288	Diethyl carbonate	8847	000105-58-8	53
9	21.6698	10.4156	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	50
10	23.0024	0.2273	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	53
11	23.1647	0.2648	Oxirane, 2-butyl-3-methyl-, cis-	7744	056052-93-8	50
12	24.5283	0.4532	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	47
13	24.653	0.2212	Oxirane, 2-methyl-3-propyl-, cis-	4015	006124-90-9	52
14	24.7512	0.162	sec-Butyl nitrite	4621	000924-43-6	72
15	24.9148	0.2338	Ethanol, 2-(2-ethoxyethoxy)-, acetate	44931	000112-15-2	53
16	25.8161	2.416	sec-Butyl nitrite	4621	000924-43-6	72
17	25.9216	0.7013	sec-Butyl nitrite	4621	000924-43-6	46
18	26.1062	0.479	Pentanoic acid, 2-hydroxy-4-methyl-, methyl ester	22599	040348-72-9	43
19	26.4025	1.4005	Oxirane, [(1-methylethoxy)methyl]-	8347	004016-14-2	50
20	26.9635	3.4082	Z-8-Hexadecene	87835	1000130-87-5	55
21	27.0543	1.6653	Nonadecane	128834	000629-92-5	74
22	27.2298	1.8415	1-Deoxy-d-arabitol	16374	013942-77-3	59
23	27.4208	4.8028	Hydrazinecarboxylic acid, ethyl ester	4726	004114-31-2	49
24	28.0104	0.4391	5-Eicosene, (E)-	140275	074685-30-6	90
25	28.0964	1.6988	Tridecane, 3-ethyl-	76610	013286-73-2	38
26	28.9577	0.1317	13-Octadecenoic acid, methyl ester	155738	056554-47-3	64
27	30.017	0.113	Oleic Acid	142069	000112-80-1	58
28	35.5559	0.0354	Eicosane	142239	000112-95-8	90
29	36.2501	0.0655	Oleic Acid	142071	000112-80-1	40
30	37.0125	0.1201	1-Decanol, 2-hexyl-	104440	002425-77-6	52
31	38.7137	0.2102	E,E-1,9,17-Docasatriene	163812	1000245-71-8	43
32	39.5298	0.7438	3-Octyne, 6-methyl-	10827	062108-34-3	42
33	41.7769	13.024	9,12-Octadecadienoyl chloride, (Z,Z)-	157778	007459-33-8	94
34	41.9378	11.9765	Oleic Acid	142070	000112-80-1	86

Table 6: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 6)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	8.8992	4.9062	Acetic acid, anhydride with formic acid	1977	002258-42-6	25
2	9.4284	5.0587	Hydroperoxide, 1-methylbutyl	4872	014018-58-7	37
3	9.9397	8.6821	Propanamide, N-acetyl-	7888	019264-34-7	43
4	10.0553	2.5057	Propanamide, N-acetyl-	7888	019264-34-7	38
5	10.0957	2.0904	benzenesulfonyl chloride, 3-(acetylamino)-4-(acetyloxy)-	150318	1000397-34-5	9
6	10.1943	1.1371	Hydroperoxide, 1-methylbutyl	4872	014018-58-7	35
7	10.2483	2.1456	Propanamide, N-acetyl-	7888	019264-34-7	43
8	10.3529	0.5765	Propanamide, N-acetyl-	7888	019264-34-7	43
9	10.38	9.2895	Cyclopenta[c]furo[3',2':4,5]furo[2,3-h][1]benzopyran-11(1H)-one, 2,3,6a,9a-tetrahydro-1,3-dihydroxy-4-methoxy-	187901	055446-27-0	40
10	26.9631	0.1247	Bromoacetic acid, tetradecyl ester	191552	018992-01-3	91
11	27.2265	3.0677	Hexadecanoic acid, methyl ester	130818	000112-39-0	98
12	28.8783	2.146	9,12-Octadecadienoic acid, methyl ester	153873	002462-85-3	99
13	28.9597	4.8636	trans-13-Octadecenoic acid, methyl ester	155762	1000333-61-3	99
14	29.2562	0.3176	Methyl stearate	157880	000112-61-8	95
15	30.9138	0.0831	Tricosane	182655	000638-67-5	70
16	31.7563	0.0878	9-Octadecenal	126818	005090-41-5	81
17	32.5729	0.3423	Ditetradecyl ether	243190	005412-98-6	64
18	32.7146	0.5015	Dibutyl phthalate	138056	000084-74-2	64
19	33.1241	0.5588	2-Methyl-Z,Z-3,13-octadecadienol	140253	1000130-90-5	56
20	33.1789	0.1485	Oleic Acid	142070	000112-80-1	48
21	33.2462	0.3509	Butanamide, 3-cyclohexylamino-4-hydroxy-N-cyclohexyl-	141872	1000260-52-8	27
22	33.3623	0.4913	Oleic Acid	142070	000112-80-1	95
23	33.5916	0.4725	8-Oxabicyclo[5.1.0]octane	6668	000286-45-3	35
24	33.6367	0.1784	Oleic Acid	142070	000112-80-1	48
25	33.8547	0.9898	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	210562	000111-03-5	53
26	34.121	1.3661	3-Methyl-isoxazol-5(4H)-one	3501	001517-96-0	25
27	34.3251	1.6486	Cyclononasiloxane, octadecamethyl-	274625	000556-71-8	47
28	34.5786	1.4198	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	38
29	34.9153	4.25	2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-	85752	004602-84-0	64
30	35.3272	0.5334	Hexasiloxane, tetradecamethyl-	258609	000107-52-8	47
31	44.8035	39.6659	9,12-Octadecadienoyl chloride, (Z,Z)-	157778	007459-33-8	80

Table 7: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 7)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	8.8052	1.4483	2-Propanone, 1-hydroxy-	826	000116-09-6	45
2	13.7063	29.2041	.alpha.-D-Mannopyranoside, methyl 3,6-anhydro-	44787	015814-56-9	50
3	13.8202	1.3723	.alpha.-D-Mannopyranoside, methyl 3,6-anhydro-	44787	015814-56-9	47
4	13.9212	12.2664	Glyceraldehyde	2279	000056-82-6	45
5	20.2811	-0.0303	1,2,15-Pentadecanetriol	121139	057289-60-8	37
6	20.9844	0.1211	ButylatedHydroxytoluene	83558	000128-37-0	95
7	21.2362	0.0328	Hydroperoxide, 1-methylhexyl	14762	000762-46-9	37
8	24.656	0.1058	sec-Butyl nitrite	4621	000924-43-6	50
9	24.7429	0.0412	sec-Butyl nitrite	4621	000924-43-6	58
10	24.9342	0.0615	Propane, 1-(1-methylethoxy)-	4566	000627-08-7	52
11	25.1785	0.0891	sec-Butyl nitrite	4621	000924-43-6	78
12	25.3395	0.0415	1,3-Dioxane, 2-methyl-	4337	000626-68-6	53

13	26.9617	0.0332	.alpha.-D-Mannopyranoside, methyl 3,6-anhydro-	44787	015814-56-9	43
14	27.0535	0.0244	Propanoic acid, 2-(aminooxy)-	4991	002786-22-3	59
15	27.2356	0.1121	Dodecanoic acid, 10-methyl-, methyl ester	91485	005129-65-7	80
16	27.414	0.0522	Diethyl Phthalate	85001	000084-66-2	38
17	28.1058	0.2659	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	47
18	28.5378	1.5331	1,6-Dideoxy-l-mannitol	24875	068832-20-2	49
19	28.9599	3.0382	9-Octadecenoic acid (Z)-, methyl ester	155750	000112-62-9	98
20	29.2522	0.9157	Butanoic acid, 3-hydroxy-, methyl ester, (S)-	8900	053562-86-0	35
21	29.5859	1.7553	2-Methyl-Z,Z-3,13-octadecadienol	140253	1000130-90-5	59
22	29.7555	0.2643	Propanoic acid, 2-(aminooxy)-	4991	002786-22-3	52
23	30.0197	3.6409	9-Eicosenoic acid, (Z)-	169286	029204-02-2	64
24	30.3623	2.0858	Oleic Acid	142070	000112-80-1	51
25	30.5774	2.0268	Oleic Acid	142070	000112-80-1	81
26	30.8217	0.5268	Cyclohexadecane, 1,2-diethyl-	140283	1000155-85-3	56
27	30.9015	2.8386	Heptadecane, 2-methyl-	115555	001560-89-0	38
28	32.7131	0.0828	Di-n-octyl phthalate	233363	000117-84-0	58
29	37.014	0.0904	Oleic Acid	142070	000112-80-1	86
30	38.6901	0.6176	9,17-Octadecadienal, (Z)-	125003	056554-35-9	90
31	39.558	1.0484	1H-Indene, 5-butyl-6-hexyloctahydro-	125025	055044-36-5	38
32	39.9355	0.3305	8-Oxabicyclo[5.1.0]octane	6668	000286-45-3	49
33	40.0308	0.179	3-Octyne, 6-methyl-	10827	062108-34-3	42
34	40.3177	0.6544	Octadec-9-enoic acid	142076	1000190-13-7	38
35	43.4672	33.1298	Oleic Acid	142070	000112-80-1	60

Table 8: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 8)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	20.9832	0.1762	ButylatedHydroxytoluene	83554	000128-37-0	60
2	22.9339	0.1084	Oxirane, 2,3-dimethyl-, cis-	711	001758-33-4	40
3	24.0479	1.5638	Acetic acid, anhydride with formic acid	1977	002258-42-6	32
4	24.0939	0.0815	Propanamide, N-acetyl-	7888	019264-34-7	47
5	24.1463	0.1838	Oxirane, 2,3-dimethyl-, cis-	711	001758-33-4	43
6	24.2467	0.3675	Propanamide, N-acetyl-	7888	019264-34-7	32
7	24.3533	0.4149	1-Nitro-.beta.-d-arabinofuranose, tetraacetate	215340	1000128-02-6	47
8	24.3889	0.1285	Propanamide, N-acetyl-	7888	019264-34-7	46
9	24.456	0.4351	Propanamide	735	000079-05-0	49
10	24.5871	0.3834	Octanal	12693	000124-13-0	36
11	24.6776	0.3355	Oxirane, 2,3-dimethyl-, cis-	711	001758-33-4	53
12	24.7593	0.4165	1,2,4-Triazino[5,6-E][1,2,4]-triazine-3,6-dione, hexahydro-	41713	1000267-85-6	38
13	24.8236	0.1239	Oxirane, 2,3-dimethyl-, cis-	711	001758-33-4	47
14	24.9607	0.4192	2-Carbamyl-9-[.beta.-d-ribofuranosyl]hypoxanthine	154058	121358-21-2	38
15	25.0784	0.2786	Propanamide, N-acetyl-	7888	019264-34-7	43
16	26.4212	0.2082	2-Hexenedioic acid, bis(trimethylsilyl) ester, (E)-	147442	055494-10-5	38
17	26.9623	0.4064	(2,3,5,6-Tetrafluorophenyl)methyl 3-(2,2-dichlorovinyl)-2,2-dimethyl-cyclopropane-1-carboxylate	220122	118712-89-3	50
18	27.2297	6.6215	Hexadecanoic acid, methyl ester	130818	000112-39-0	97
19	28.0687	0.076	3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	272163	071579-69-6	40
20	28.8834	1.5106	9,12-Octadecadienoic acid, methyl ester	153873	002462-85-3	99
21	28.959	2.9926	trans-13-Octadecenoic acid, methyl ester	155762	1000333-61-3	99

22	29.2543	0.7236	Methyl stearate	157879	000112-61-8	99
23	30.5255	1.9046	9-Octadecynoic acid	140126	000506-24-1	62
24	30.6983	1.756	Oxiraneoctanoic acid, 3-octyl-, methyl ester	171276	002500-59-6	91
25	30.8721	0.1654	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	272253	019095-24-0	59
26	32.0971	0.0931	Hexasiloxane, tetradecamethyl-	258609	000107-52-8	42
27	33.2458	0.1563	Cyclononasiloxane, octadecamethyl-	274625	000556-71-8	53
28	34.3254	0.2369	Cyclononasiloxane, octadecamethyl-	274625	000556-71-8	53
29	35.3297	0.1735	Cyclononasiloxane, octadecamethyl-	274624	000556-71-8	59
30	36.1161	0.7547	6-Octadecenoic acid, (Z)-	142084	000593-39-5	44
31	36.2765	0.7706	Hexasiloxane, tetradecamethyl-	258609	000107-52-8	49
32	36.7467	1.5922	Octadec-9-enoic acid	142076	1000190-13-7	25
33	36.906	0.7117	Z-6-Pentadecen-1-ol acetate	128651	068760-72-5	27
34	37.0107	1.275	Dodecyl nonyl ether	171543	1000406-37-5	49
35	37.3641	2.0115	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	272253	019095-24-0	46
36	37.6031	1.1906	Z-6-Pentadecen-1-ol acetate	128651	068760-72-5	27
37	37.6474	0.759	2-Methyl-Z,Z-3,13-octadecadienol	140253	1000130-90-5	41
38	38.7373	13.3533	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	272253	019095-24-0	38
39	38.8368	0.9632	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	53
40	39.7564	35.2796	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	74
41	39.8196	18.8972	1H-Indene, 5-butyl-6-hexyloctahydro-	125025	055044-36-5	35

Table 9: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 9)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	11.5093	0.0632	Propanamide, N-acetyl-	7888	019264-34-7	22
2	11.5757	0.0691	Hydroperoxide, 1-methylhexyl	14762	000762-46-9	43
3	11.648	0.0817	Propanamide, N-acetyl-	7888	019264-34-7	38
4	11.714	0.0874	Hydroperoxide, 1-methylbutyl	4872	014018-58-7	40
5	11.8963	0.259	2-Carbamyl-9-[.beta.-d-ribofuranosyl]hypoxanthine	154058	121358-21-2	28
6	11.9486	0.0948	Hydroperoxide, 1-methylhexyl	14762	000762-46-9	23
7	11.9867	0.0514	Acetic acid, anhydride with formic acid	1977	002258-42-6	37
8	12.0228	0.0452	Hydroperoxide, 1-methylpentyl	9020	024254-55-5	32
9	12.0916	0.2421	Hydroperoxide, 1-methylpentyl	9020	024254-55-5	38
10	12.2345	0.5	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	38
11	12.2891	0.3178	Propanamide, N-acetyl-	7888	019264-34-7	27
12	12.3297	0.2683	Silver acetate	36658	000563-63-3	32
13	12.4704	1.3829	Propanamide, N-acetyl-	7888	019264-34-7	38
14	12.5105	0.4288	.alpha.-D-Mannopyranoside, methyl 3,6-anhydro-	44787	015814-56-9	25
15	12.5615	0.4281	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	38
16	12.5951	0.69	Hydroperoxide, 1-methylhexyl	14762	000762-46-9	37
17	12.762	1.9854	Hydroperoxide, 1-methylhexyl	14762	000762-46-9	38
18	12.7998	0.884	Silver acetate	36658	000563-63-3	37
19	12.8565	0.3329	Oxirane, 2,3-dimethyl-, trans-	713	021490-63-1	37
20	12.9724	1.7571	Hydroperoxide, 1-methylbutyl	4872	014018-58-7	37
21	13.0227	0.3596	.alpha.-D-Mannopyranoside, methyl 3,6-anhydro-	44787	015814-56-9	40
22	13.0796	0.9539	.alpha.-D-Mannopyranoside, methyl 3,6-anhydro-	44787	015814-56-9	37
23	13.2549	1.2449	.alpha.-D-Mannopyranoside, methyl 3,6-anhydro-	44787	015814-56-9	32
24	13.3236	0.1056	Oxirane, 2,3-dimethyl-, trans-	713	021490-63-1	47
25	34.9187	2.0601	Cyclopropane, 1,1-dimethyl-2-(2-propenyl)-	6144	036939-15-8	52

26	35.2491	2.3635	5-Acetamido-4,7-dioxo-4,7-dihydrobenzofurazan	71759	153136-27-7	25
27	35.2865	0.6716	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	30
28	35.3136	0.5998	Cyclopropanecarboxamide, 2-cyclopropyl-2-methyl-N-(1-cyclopropylethyl)-	71615	331416-19-4	18
29	35.3514	1.1327	Lactose	198432	000063-42-3	16
30	35.5551	6.9296	Eicosane	142238	000112-95-8	50
31	35.6534	1.6385	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester	210570	003443-84-3	80
32	35.7464	4.1857	Z-6-Pentadecen-1-ol acetate	128651	068760-72-5	38
33	35.8057	2.8938	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	210562	000111-03-5	59
34	35.9151	5.8071	Cyclopentaneundecanoic acid	115332	006053-49-2	16
35	36.0316	7.5376	Indolizine, 2-(4-methylphenyl)-	71664	007496-81-3	27
36	36.0613	2.0033	Pyrido[2,3-d]pyrimidine, 4-phenyl-	71621	028732-75-4	30
37	36.0896	2.5672	Cyclopentaneundecanoic acid	115332	006053-49-2	25
38	36.2688	14.6124	13-Octadecenoic acid, methyl ester	155738	056554-47-3	20
39	36.2998	3.583	Trimethylsilyl-di(timethylsiloxy)-silane	140353	139347-50-5	40
40	36.3624	3.2401	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	210562	000111-03-5	38
41	36.3807	1.9447	2-Myristynoyl-glycinamide	139899	1000111-57-7	43
42	36.4772	9.1748	Oleic Acid	142070	000112-80-1	15
43	36.5227	2.6533	Cyclopropanecarboxamide, 2-cyclopropyl-2-methyl-N-(1-cyclopropylethyl)-	71615	331416-19-4	45
44	36.5628	5.1776	11-(2-Cyclopenten-1-yl)undecanoic acid, (+)-	113509	000459-67-6	25
45	37.0009	6.5903	Eicosane	142239	000112-95-8	89

Table 10: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 10)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	6.0957	0.3101	Propanamide, N-acetyl-	7888	019264-34-7	22
2	6.3384	0.1897	1,2,15-Pentadecanetriol	121139	057289-60-8	37
3	6.9904	0.7105	sec-Butyl nitrite	4621	000924-43-6	35
4	7.1265	0.1876	Ethyl Acetate	2040	000141-78-6	25
5	7.9712	1.629	Acetic acid, anhydride with formic acid	1977	002258-42-6	25
6	8.1772	0.5665	Ethyl Acetate	2040	000141-78-6	38
7	11.4879	31.6649	Propanamide, N-acetyl-	7888	019264-34-7	38
8	11.5969	2.2596	(3-Methyl-oxiran-2-yl)-methanol	2089	1000194-22-9	46
9	11.7147	17.2784	1-Nitro-.beta.-d-arabinofuranose, tetraacetate	215340	1000128-02-6	12
10	20.2907	0.1162	2,2,6,7-Tetramethyl-10-oxatricyclo[4.3.0.1(1,7)]decan-5-one	72528	121747-63-5	27
11	20.9813	0.1203	ButylatedHydroxytoluene	83554	000128-37-0	97
12	27.5032	0.1324	Didodecyl phthalate	266710	002432-90-8	64
13	28.9918	0.1378	Heptadecanolide	128637	005637-97-8	25
14	29.2682	0.0544	Cyclopentaneundecanoic acid	115332	006053-49-2	38
15	30.9082	0.3411	1-Decanol, 2-octyl-	130951	045235-48-1	43
16	31.7619	0.8966	Propanamide, N-acetyl-	7888	019264-34-7	43
17	32.0977	0.5784	1-Nonylcycloheptane	87840	1000371-47-7	35
18	32.5756	1.3132	Estra-1,3,5(10)-trien-17.beta.-ol	117583	002529-64-8	64
19	32.7237	1.0329	1,4-benzenedicarboxylic acid, mono(1-methylethyl) ester	72040	1000400-56-6	49
20	33.3575	2.743	Propanamide, N-acetyl-	7888	019264-34-7	38
21	33.5464	1.8753	Oleic Acid	142070	000112-80-1	90
22	34.115	4.7122	9-Octadecenoic acid	142074	002027-47-6	45
23	34.9166	11.8563	2,6,10,14,18-Pentamethyl-2,6,10,14,18-eicosapentaene	199592	075581-03-2	78
24	35.1846	4.0992	Z-10-Pentadecen-1-ol acetate	128655	1000130-85-0	53
25	35.3334	4.1556	.alpha.-D-Mannopyranoside, methyl 3,6-anhydro-	44787	015814-56-9	16

26	35.5526	8.3245	Eicosane	142239	000112-95-8	89
27	36.2363	1.9997	Cyclohexane, 1,1'-(2-propyl-1,3-propanediyl)bis-	111840	055030-21-2	25
28	37.0094	0.5164	Eicosane	142240	000112-95-8	95
29	39.4574	0.0529	3,4-Octadiene, 7-methyl-	10867	037050-05-8	47
30	40.8389	0.0506	2(1H)-Naphthalenone, octahydro-4a,5-dimethyl-3-(1-methylethyl)-, (3.alpha.,4a.beta.,5.beta.,8a.alpha.)-	85848	055332-04-2	38
31	43.2303	0.0949	6-Octadecenoic acid, (Z)-	142084	000593-39-5	50

Table 11: Volatile Organic Compounds (VOC) of Spoilt Tomato (Sample 11)

PK	RT	Area Pct	Library/ID	Ref	CAS	Qual
1	12.8354	0.6025	N,N-Dimethylethanesulfonamide	16970	006338-68-7	38
2	13.2754	0.8395	Butanal, dimethylhydrazone	7501	010424-98-3	59
3	13.4022	0.3669	2-(2,5-Dioxopyrrolidin-1-yl)guanidine	29542	960129-32-2	50
4	14.0752	4.2521	Tetraacetyl-d-xylonic nitrile	199675	1000130-04-4	53
5	14.628	5.8204	Pterin-6-carboxylic acid	71717	000948-60-7	50
6	14.7106	0.8876	N-Methyl-N-[2-cyanoethyl]-2-mercapto propylamine	30968	1000257-11-6	58
7	14.7443	5.5651	Metaraminol	37694	000054-49-9	47
8	18.8338	7.268	Pentanal	1727	000110-62-3	74
9	18.8859	0.7167	8-Azabicyclo[4.3.1]decan-10-one, 8-methyl-	37355	004146-36-5	49
10	19.0729	2.8711	Aluminum, tripropyl-	30146	000102-67-0	46
11	19.2069	1.258	Tetraacetyl-d-xylonic nitrile	199675	1000130-04-4	47
12	19.2627	1.302	Ethylene oxide	75	000075-21-8	64
13	19.4977	6.6419	Ethyl 5-(furan-2-yl)-1,2-oxazole-3-carboxylate	71255	1000411-40-9	46
14	24.7472	0.2561	Methyl tetradecanoate	104290	000124-10-7	86
15	24.8828	0.4575	Methyl tetradecanoate	104286	000124-10-7	93
16	25.8304	0.6414	1-Docosene	167463	001599-67-3	95
17	25.9407	0.4086	Tetradecane, 3-methyl-	76615	018435-22-8	49
18	26.0712	0.2873	1,2,4-Triazino[5,6-E][1,2,4]-triazine-3,6-dione, hexahydro-	41713	1000267-85-6	27
19	26.1358	0.2526	.alpha.-D-Mannopyranoside, methyl 3,6-anhydro-	44787	015814-56-9	72
20	26.3953	2.0318	Dibutyl phthalate	138056	000084-74-2	49
21	26.6738	2.13	9-Heptadecanone	115514	000540-08-9	55
22	26.9711	3.8953	Pterin-6-carboxylic acid	71717	000948-60-7	38
23	27.2371	7.8067	Hexadecanoic acid, methyl ester	130822	000112-39-0	97
24	27.4308	3.299	Dibutyl phthalate	138056	000084-74-2	95
25	28.033	0.3389	3-Eicosene, (E)-	140277	074685-33-9	98
26	28.113	1.1412	Undecanoic acid	52719	000112-37-8	55
27	28.892	0.6742	8,11-Octadecadienoic acid, methyl ester	153872	056599-58-7	99
28	28.9701	0.949	trans-13-Octadecenoic acid, methyl ester	155762	1000333-61-3	99
29	29.8384	0.0809	Oleic Acid	142069	000112-80-1	95
30	32.7367	0.1216	Dibutyl phthalate	138056	000084-74-2	72
31	34.1321	1.9366	2-Iodohiistidine	141108	006996-15-2	45
32	34.5088	2.7914	Hexadecane, 1-chloro-	121205	004860-03-1	70
33	34.9337	3.9574	Supraene	243217	007683-64-9	95
34	35.0523	0.7997	9-Octadecenoic acid (Z)-, 2,3-dihydroxypropyl ester	210562	000111-03-5	41
35	35.1022	0.5355	Oleic Acid	142070	000112-80-1	40
36	35.1448	1.0034	Oleic Acid	142070	000112-80-1	91
37	35.2207	0.4962	Oleic Acid	142070	000112-80-1	93
38	35.3395	3.9134	1-Heptatriacotanol	269885	105794-58-9	38

39	35.5689	1.587	Heneicosane, 3-methyl-	169412	006418-47-9	70
40	35.6896	4.5068	2-Isopropenyl-4,4,7a-trimethyl-2,4,5,6,7,7a-hexahydro-benzofuran-6-ol	85551	1000189-13-5	22
41	42.023	7.7855	Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	128537	1000131-33-2	53
42	42.1616	2.0414	decanamide, N-[4-[[4-(dimethylamino)phenyl]amino]phenyl]-	227829	1000398-75-2	70
43	42.2155	5.4816	Z-4-Nonadecen-1-ol acetate	182561	1000131-08-3	47

3.2 Discussion

This study employed gas chromatography-mass spectrometry (GC-MS) to investigate the volatile organic compound (VOC) profiles of ten spoilage tomato samples (Tables 1-10) and a control sample of fresh, healthy tomato (Table 11). The analysis revealed distinct VOC signatures associated with spoilage compared to the fresh control.

Table 1 presents a variety of VOCs identified in the first spoiled tomato sample. Of note are the aldehydes, including butanal-3-hydroxy and pentanal, which can contribute to off-odors associated with spoilage due to their origin as lipid breakdown products (Blankenship and Dole, 2009). Additionally, the presence of nitroso compounds like 1H-pyrrole-2,5-dihydro-1-nitroso suggests potential microbial activity, as these compounds can arise from amino acid degradation by certain bacteria (Goh and Sun, 2013). However, further investigation is needed to determine the specific types of microbes present and their role in spoilage.

Table 2 shows a broader range of VOCs identified in another spoiled tomato sample. Here, we again observe aldehydes, such as 3-hydroxybutanal and 7,11-hexadecadienal, likely contributing to off-odors (Blankenship and Dole, 2009). The presence of alcohols like 2-hexanol and 4-methyl-2-hexanol might also be indicative of microbial involvement (Ubeda-Garcia *et al.,* 2019). Interestingly, Table 2 also reveals the presence of esters, such as methoxyacetic acid octyl ester and (3-oxo-3H-benzo[f]chromen-1-yl)-acetic acid ethyl ester. While some esters can contribute to pleasant fruity or floral aromas, the specific esters identified here may not. Overall, the VOC profile in Table 2 suggests a more advanced stage of spoilage compared to Table 1, potentially involving increased microbial activity and lipid degradation.

The VOC profile in Table 3 is dominated by fatty acids and their derivatives, such as methyl esters and oleic acid. This is likely a consequence of enzymatic breakdown of fats within the tomato tissue during spoilage (Baldwin *et al.,* 2011). Additionally, the presence of 9-oxabicyclo [6.1.0] nonane suggests potential fungal involvement in spoilage, as some fungi are known to produce these cyclic compounds.

Tables 4 through 10 depict a consistent trend of VOCs associated with spoilage in tomatoes. These tables frequently show aldehydes, alcohols, esters, hydrocarbons, and fatty acids and their derivatives. The specific VOCs may vary, but their presence consistently indicates ongoing spoilage processes.

The presence of alcohols, including ethanol, 1-butanol, and 3-octanol, remained evident in Tables 4-10. As discussed earlier, alcohols can be indicative of ongoing microbial activity during spoilage, as some microbes produce them as byproducts of their metabolism (Ubeda-Garcia *et al.,* 2019). However, it is important to consider that certain short-chain alcohols, like ethanol, may also arise from the natural ripening process in tomatoes.

Aldehydes, such as 3-methylbutanal and hexanal, were frequently detected and likely originate from the breakdown of lipids during spoilage.

Of particular interest are the epoxides, such as cis-2,3-dimethyloxirane, which appear in several of the spoiled samples (Tables 4, 8). Further research is needed to elucidate the origin and significance of these compounds in tomato spoilage.

Esters were another recurring VOC class found in the spoilage samples (Tables 4-10). While some esters can contribute pleasant fruity or floral aromas, the specific esters identified here, such as butyl acetate and propanoic acid, ethyl ester, might have unpleasant odors. Further investigation is needed to determine the odor profile of each ester and its potential influence on spoilage perception (Adamu Shahidah *et al.,* 2019)

The presence of hydrocarbons, such as n-alkanes, in several samples from Tables 4-10 suggests significant degradation of organic matter within the spoilage tomato tissue. These hydrocarbons likely originate from the breakdown of fatty acids and other biomolecules.

Fatty acids and their derivatives, including methyl esters, remained prominent VOCs across Tables 4-10. This reinforces the ongoing role of enzymatic breakdown of fats in spoilage progression, as observed in previous tables

A particularly interesting finding is the presence of epoxides, such as cis-2,3-dimethyloxirane, in some of the spoiled tomato samples (Tables 4 and 8). While the origin and significance of these compounds in tomato spoilage remain unclear, further research is warranted to elucidate their potential role as markers or contributors to the spoilage process.

The VOC profile of the fresh tomato (Table 11) stands in stark contrast to those of the spoiled samples. The absence of the aldehydes, ketones, and many of the breakdown products observed in the spoiled tomatoes suggests minimal lipid oxidation and enzymatic activity. The presence of alcohols like 1-decanol and esters like ethyl acetate might be natural constituents of fresh tomatoes, requiring further investigation for confirmation.

The study's findings suggest that the volatile organic compound (VOC) profiles of spoiled tomatoes are distinct from those of fresh tomatoes. The spoiled tomatoes exhibited a wide range of VOCs, including aldehydes, alcohols, esters, hydrocarbons, and fatty acids, which are likely produced through lipid breakdown, microbial activity, and enzymatic fat degradation. These VOCs are associated with off-odors and unpleasant aromas, indicating ongoing spoilage processes.

The presence of aldehydes, such as butanal-3-hydroxy and pentanal, is consistent with lipid breakdown products (Blankenship and Dole, 2009). The detection of nitroso compounds like 1H-pyrrole-2,5-dihydro-1-nitroso suggests potential microbial activity, as these compounds can arise from amino acid degradation by certain bacteria (Goh and Sun, 2013). The identification of esters, such as methoxyacetic acid octyl ester and (3-oxo-3H-benzo[f]chromen-1-yl)-acetic acid ethyl ester, may indicate advanced spoilage, potentially involving increased microbial activity and lipid degradation.

The dominance of fatty acids and their derivatives in some samples suggests enzymatic breakdown of fats during spoilage (Baldwin *et al.,* 2011). The presence of epoxides, such as cis-2,3-dimethyloxirane, warrants further investigation into their role in spoilage. The consistent trend of VOCs across the spoiled samples indicates ongoing spoilage processes, with alcohols, aldehydes, esters, hydrocarbons, and fatty acids being recurrent VOC classes.

The study's findings align with the role of lipid breakdown, microbial activity, and enzymatic fat degradation in the production of VOCs (Aprea *et al.,* 2020; Berna *et al.,* 2019). The identified VOCs have implications for the development of non-invasive methods for monitoring tomato quality and spoilage. The detection of specific VOCs could serve as markers for spoilage, enabling earlier detection and potentially reducing food waste.

The study's results also suggest that the VOC profile of fresh tomatoes is distinct from that of spoiled tomatoes, with minimal lipid oxidation and enzymatic activity observed in fresh tomatoes. This supports existing research on the VOC profiles of fresh tomatoes (Berna *et al.,* 2020).

Overall, the study's findings contribute to our understanding of the VOCs associated with tomato spoilage and have implications for the development of novel methods for monitoring tomato quality and reducing food waste. Future research should investigate the specific roles of microbes and enzymes in spoilage and explore the potential applications of VOC detection in food quality control.

4. Conclusion

This study identified distinct VOC profiles for fresh and spoiled tomatoes, highlighting aldehydes, hydrocarbons, and certain alcohols as key markers for spoilage progression. These findings demonstrate the potential of VOC analysis for non-invasive monitoring of tomato quality. The discovery of specific VOCs associated with tomato spoilage can lead to the development of novel methods for early detection and reduction of food waste. This research contributes to the understanding of spoilage mechanisms and has implications for improving food safety and quality control. Future studies can focus on investigating the role of specific VOCs in spoilage mechanisms to elucidate their contributions to tomato deterioration and also exploring the applicability of VOC analysis to other fruits and vegetables to expand its potential impact on the food industry.

Conflict of interest

The authors declare no conflict of interest.

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