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Comparative Head Space GC/MS Studies of Different Flavored Moâssel in the Egyptian Market (II)

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Abstract

This study designed to investigate three various samples of Egyptian Moâssel (flavored tobacco) used in water pipe smoking. The specimens (Guava, Mixed Fruits and Watermelon) were collected from the Egyptian market, which were produced by Al Dandash company (Egyptian famed tobacco company). They were examined by Head Space GC/MS. There were relatively differences among the investigated specimens. The identified compounds of the first one (Guava) exhibited 31 ingredients, which represented (81.38 %) of the compounds. The main one was fraistone (12.87 %). While, the second one (Mixed Fruits) specimen displayed 36 recognized compounds, which represented (91.98 %) of the sample components. The main constituent was isoamyl acetate (19.83 %). Finally, the last one (Watermelon) exhibited 27 identified ingredients, which represented (68.60 %) of the total compounds and the highest compound was 1,2-propanediol (25.23 %) of the constituents.

Key words

Egyptian Flavored Moâssel, Head Space GC/MS, Al Dandash Company

1. Introduction

Smoking of Tobacco is a serious and addictive habit. In the UK, half of all lifelong cigarette smokers died due to smoking [1]. Moreover, smokers reduced an average of around 3 months of life expectation for every year smoked after the age of 35; in sustained smokers this amounts to a total loss of around 10 years of lifetime [1, 2]. Furthermore, passive inhalation of the smoke harms others [3, 4]. One of tobacco smoking types is Shisha. It has many alternative names such as Hookah or water pipe or hubble bubble. In the Middle Eastern region, it is an ancient type of non-cigarette tobacco smoking that has been generally found. Hookah smoke has more than 4800 numerous substances. Many of them are carcinogens and tumor promoters [5-7]. By reviewing the literature, three flavored Moâssel used in the Egyptian Hookah were analyzed by Head Space GC/MS. They showed great difference in some of them in their composition. Consequently, the harmful effects may be varied from one sample to another [8]. Therefore, the authors provoked to analyze other samples of flavored Moâssel used in in the Egyptian Hookah by Head space GC/MS.

2. Materials and Methods

2.1. Materials

Flavored Egyptian Moâssel specimens *viz.*, Guava (GFM), Mixed Fruits (MixFFM) and Watermelon (WFM) were collected June 2016 from the Egyptian market. The samples were produced in Egypt by Al Dandash Company.

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2.2. Method

Shimadzu GC/MS with Head Space system provided by FID (Flame Ionization Detector), connected to the Mass Spectrometer Model: QP2010Ultra. Total GLC chromatograms and mass spectra were recorded in the electron impact ionization mode at 70 eV, using ACQ Mode of scan from 35 to 500 m/z in 0.3 s. The used column was 0.25 mm in internal diameter, 30 m length, packed with Rtx-MS and 0.25 μm film thickness. The injected volume was 1.0 μl, using helium as carrier gas at flow rate 40 ml/min. The analyses were carried out at a programmed temperature; the initial temperature was 40 °C (Kept for 2 min), then increased at a rate 30-50 °C to the final temperature 210 °C (kept for 5 min). Injector and detector had the same temperature 230 °C. The total run time was 45 min and split ratio 1:50 [8].

3. Results

Head Space GC/MS analyses

The qualitative analysis was done by direct comparison of and fragmentation patterns of the identified compounds with archive mass spectra lipid library and quantitation was based on peak area integration [9, 10].

3.1. GFM analysis

GFM exhibited 38 compounds from Head Space GC/MS analysis. The unidentified compounds represented 18.62 % (7 compounds) and identified compounds represented 81.38 % (31 compounds). The major one was fraistone (12.87 %). All identified compounds are oxygenated as shown in **(Figure 1)** and enumerated in **(Table 1)**.

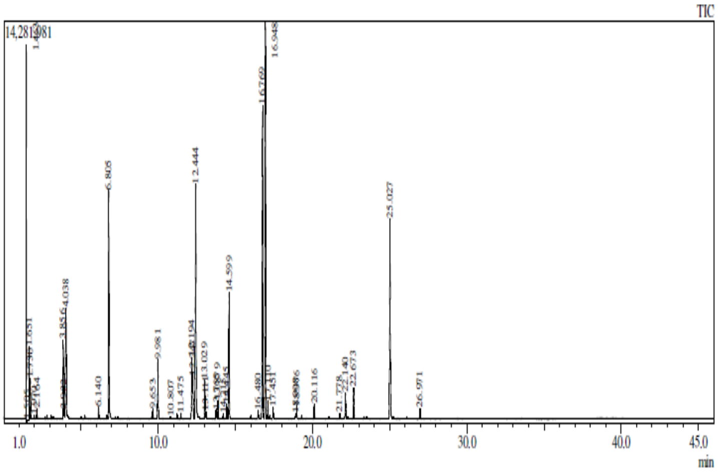

Figure 1: Total ion GC chromatogram of GFM.

3.2. MixFFM analysis

Qualitative analysis of MixFFM exhibited 39 compounds using Head Space GC/MS. The unidentified compounds represented 08.02 % (3 compounds) and identified compounds represented 91.98 % (36 compounds). The major one was isoamyl acetate (19.83 %). The identified compounds are classified into two classes *viz*., 86.67 % oxygenated and 05.31 % hydrocarbons compounds as shown in **(Figure 2)** and enumerated in **(Table 2)**.

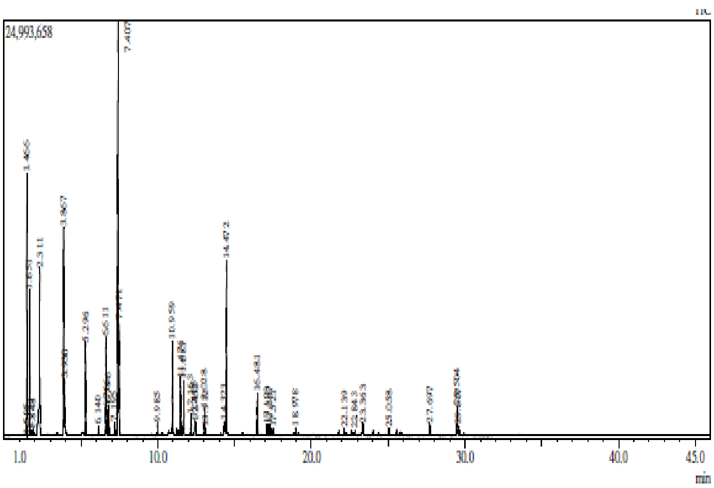

Figure 2: Total ion GC chromatogram of MixFFM.

3.3. WFM analysis

Qualitative analysis WFM exhibited 37 compounds by Head Space GC/MS. The unidentified compounds represented 31.40 % (10 components). The identified compounds represented 68.60 % (27 ingredients). The chief one was 1,2-propanediol (25.23 %). The recognized components are classified into three various classes *viz*., 60.57 % oxygenated, 04.76 % nitrogenous and 03.27 % hydrocarbons compounds as displayed in **(Figure 3)** and listed in **(Table 3)**.

4. Discussion

The current study investigated three different flavored Egyptian Moâssel *viz*., GFM, MixFFM and WFM by Head Space GC/MS analyses. The samples exhibited very high ratio of oxygenated constituents and traces of (nitrogenous & hydrocarbons) constituents. Therefore, they are powerful flavored samples.

The three samples contained seven common compounds *viz*., 5,6-epoxy-*β*-ionone, acetone, acetic acid, 3-methyl-1-butanol, furfural, *Z*-3-hexen-1-ol and benzyl alcohol.

Furthermore, GFM and MixFFM had also seven common compounds *viz*., 2-methyl-1-butanol, benzaldehyde, *Z*-3-hexenyl acetate, linalool, benzyl acetate, eugenol, *E*-methyl cinnamate. While, GFM and WFM had three common compound; hexanoic acid, anethole and benzyl butanoate. Finally, MixFFM and WFM had one more common compound (isoamyl butyrate). From the aforementioned data, there are relatively differences among the three studied samples, specially between (WFM & MixFFM). But, GFM and MixFFM samples are the most similar samples.

Fraistone (12.87 %) was the major compound in GFM sample. It is colorless liquid with fresh fruity odor. It considered being raw material of manufacturing floral fragrances [11]. Flavor esters compounds have a great commercial importance due to their application chiefly in cosmetic and food industries. Also, they are environmentally benign-solvents and intermediates in pharmaceutical and chemical processes. The most wanted flavor in food industries, are the alkyl esters. Specially, isoamyl acetate due to its strong banana flavor [12]. It is the main compound in MixFFM sample (19.83 %). It is widely used as a flavoring compound in a variety of foodstuffs, such as butterscotch, honey, beverages and artificial coffee [13].

Furthermore, it is also one of the major flavor substance of fermented alcoholic beverages (sake, beer & wines) [13]. On the other hand, it has an irritant and central nervous system depressant effect. Moreover, exposure to concentrations (950 ppm for 30 minutes) caused irritation of the nose & eyes, weakness, headaches, vertigo, palpitations, gastrointestinal disorders, anemia, cutaneous lesions and dermatitis [14]. It may undergo enzymatic hydrolysis to form acetic acid and isoamyl alcohol. Five acetate esters including isoamyl acetate were administered orally to rabbits to study the mechanism of drunkenness. The ester administration reduced the blood pO_2 and pCO_2 [15-17].

The enzymic hydrolysis of isoamyl acetate was studied *in vitro* with preparations of pancreatic and whole homogenates of pig jejunum. Incubation of pancreatin with 500 µl/l isoamyl acetate and pig jejunum resulted in 100 % hydrolysis. Therefore, it was presumed that those esters hydrolyzed rapidly *in vitro* would also be degraded readily in the animal [15-17].

Finally, the third one WFM showed that 1,2-propanediol (25.23 %) was the main constituents. The 1,2-propanediol (undiluted) was slightly irritating to the eye and producing mild transient conjunctivitis. The eye recovered after the contact removed [18]. Its concentration augmented the hazard of respiratory and immune illnesses in children with hay fever, asthma, allergies and eczema from 50 % to 180 % [19, 20]. The structures of the three main ingredients in the samples are shown in **(Figure 4)**.

Table 1: Identified compounds of GFM from Head Space GC/MS.

No.	Name	RT*	RRT**	Base peak	Relative Area %	M. Weight	M. Formula
1	5,6-Epoxy-β-ionone	01.46	0.087	40	06.20	208	$C_{13}H_{20}O_2$
2	Ethyl lactate	01.65	0.098	45	01.42	118	$C_5H_{10}O_3$
3	Acetone	01.73	0.103	43	01.20	58	C_3H_6O
4	Butanal (syn.: Butyraldehyde)	01.97	0.118	43	00.31	72	C_4H_8O
5	Acetic acid	02.16	0.129	43	00.71	60	$C_2H_4O_2$
6	3-Methyl-1-butanol (Fusel oil)	03.85	0.230	55	02.25	88	$C_5H_{12}O$
7	2-Methyl-1-butanol	03.93	0.234	57	00.28	88	$C_5H_{12}O$
8	1,2-Propanediol	04.04	0.241	45	05.50	76	$C_3H_8O_2$
9	Furfural	06.14	0.366	96	00.43	96	$C_5H_4O_2$
10	*Z*-3-Hexen-1-ol	06.80	0.406	41	08.60	100	$C_6H_{12}O$
11	Ethyl acetoacetate	09.65	0.576	43	00.38	130	$C_6H_{10}O_3$
12	Benzaldehyde	09.98	0.595	77	02.35	106	C_7H_6O
13	Hexanoic acid	10.80	0.644	60	00.17	116	$C_6H_{12}O_2$
14	*Z*-3-Hexenyl acetate	11.47	0.684	43	00.20	142	$C_8H_{14}O_2$
15	2-Ethyl-1-hexanol	12.19	0.727	57	02.98	130	$C_8H_{18}O$
16	1,8-Cineole (syn.: Eucalyptol)	12.24	0.730	43	01.56	154	$C_{10}H_{18}O$
17	Benzyl alcohol	12.44	0.742	79	12.17	108	C_7H_8O
18	Isoamy butyrate (syn.: Butanoic acid, 3-methylbutyl ester)	13.03	0.777	71	01.37	158	$C_9H_{18}O_2$
19	Amyl butyrate (syn.: Pentyl butanoate)	13.11	0.782	71	00.25	158	$C_9H_{18}O_2$
20	4-Methyl-2-pentyl, 1,3 dioxolane	13.88	0.828	87	00.64	158	$C_9H_{18}O_2$
21	Linalool	14.44	0.862	71	00.60	154	$C_{10}H_{18}O$
22	Isoamyl isovalerate (syn.: Apple oil)	14.59	0.871	70	04.50	172	$C_{10}H_{20}O_2$
23	Benzyl acetate	16.48	0.983	108	00.33	150	$C_9H_{10}O_2$
24	Fraistone (syn.: Ethyl (2,4-Dimethyl-1,3-dioxolan-2-yl) acetate)	16.76	1.000	43	12.87	188	$C_9H_{16}O$
25	*Z*-3-Hexenyl butyrate	17.11	1.021	67	00.62	170	$C_{10}H_{18}O_2$
26	Methyl salicylate	17.45	1.041	120	00.47	152	$C_8H_8O_3$
27	Anethole	20.11	0.200		00.60	148	$C_{10}H_{12}O$
28	Benzyl butanoate	21.78	0.300	91	00.27	178	$C_{11}H_{14}O_2$
29	Eugenol	22.14	0.321	164	01.13	164	$C_{10}H_{12}O_2$
30	*Z*-3-Hexenyl hexoate	22.67	0.353	82	01.20	198	$C_{12}H_{22}O_2$
31	*E*-Methyl cinnamate	25.02	1.493	31	09.82	176	$C_{11}H_{12}O_2$
Unidentified compounds 18.62 %							
Identified compounds	**81.38 %**	Oxygenated compounds					

***RT:** Retention Time. ****RRT:** Relative Retention Time.

Table 2: Identified compounds of MixFFM from Head Space GC/MS.

No.	Name	RT*	RRT**	Base peak	Relative Area %	M. Weight	M. Formula
1	5,6-Epoxy-*β*-ionone	1.46	0.197	39	6.11	208	$C_{13}H_{20}O_2$
2	Ethanol	1.65	0.222	45	2.70	46	C_2H_6O
3	Acetone	1.73	0.223	43	0.37	58	C_3H_6O
4	Acetic acid	1.85	0.250	43	0.41	60	$C_2H_4O_2$
5	Dihydrolinalool	2.31	0.312	43	4.59	88	$C_4H_8O_2$
6	3-Methyl-1-butanol (Fusel oil)	3.86	0.521	55	8.15	88	$C_5H_{12}O$
7	2-Methyl-1-butanol	3.93	0.531	41	2.44	88	$C_5H_{12}O$
8	Ethyl butanoate (syn.: Ethyl butyrate)	5.29	0.714	71	3.56	116	$C_6H_{12}O_2$
9	Furfural	6.14	0.829	96	0.42	96	$C_5H_4O_2$
10	Ethyl-2-methyl butanoate	6.61	0.893	57	3.99	130	$C_7H_{14}O_2$
11	Ethyl-3-methyl butanoate	6.70	0.905	88	1.07	130	$C_7H_{14}O_2$
12	*Z*-3-Hexen-1-ol	6.79	0.917	41	1.44	100	$C_6H_{12}O$
13	*n*-Hexyl formate	7.19	0.971	56	0.72	130	$C_7H_{14}O_2$
14	Isoamyl acetate	7.40	1.000	43	19.83	130	$C_7H_{14}O_2$
15	2-Methyl butyl acetate	7.47	1.009	43	4.54	130	$C_7H_{14}O_2$
16	Benzaldehyde	9.98	1.348	77	0.64	106	C_7H_6O
17	Myrcene	10.95	1.479	41	4.31	136	$C_{10}H_{16}$
18	*Z*-3-Hexenyl acetate	11.47	1.550	43	2.70	142	$C_8H_{14}O_2$
19	*n*-Hexyl acetate	11.68	1.578	43	2.62	144	$C_8H_{16}O_2$
20	Limonene	12.16	1.643	68	1.00	136	$C_{10}H_{16}$
21	Benzyl alcohol	12.40	1.675	79	0.83	108	C_7H_8O
22	Isoamyl butyrate	13.02	1.759	71	1.61	158	$C_9H_{18}O_2$
23	Glycerol monoacetate	14.32	1.935	43	0.96	134	$C_5H_{10}O_4$
24	Linalool	14.47	1.955	71	9.79	154	$C_{10}H_{18}O$
25	Benzyl acetate	16.48	2.227	108	0.20	150	$C_9H_{10}O_2$
26	*Z*-3-Hexenyl butyrate	17.10	2.310	67	0.55	170	$C_{10}H_{18}O_2$
27	Hexyl butanoate	17.26	2.332	43	0.61	172	$C_{10}H_{20}O_2$
28	Ethyl maltol	17.52	2.367	140	0.42	140	$C_7H_8O_3$
29	Isoamyl caproate	18.98	2.564	70	0.42	186	$C_{11}H_{22}O_2$
30	Eugenol	22.14	2.991	164	0.41	164	$C_{10}H_{12}O_2$
31	*E*-Methyl cinnamate	22.84	3.086	131	0.33	162	$C_{10}H_{10}O_2$
32	Diphenylether	23.36	3.156	170	0.87	170	$C_{12}H_{10}O$
33	*γ*-Decalactone	25.06	3.386	85	0.42	170	$C_{10}H_{18}O_2$
34	*γ*-Undecalactone	27.69	3.741	85	0.74	184	$C_{11}H_{20}O_2$
35	Jasmal	29.30	3.986	129	1.67	214	$C_{12}H_{22}O_3$
36	Dihydro methyl jasmonate	29.60	4.000	83	0.54	226	$C_{13}H_{22}O_3$

Unidentified compounds 08.02%

Identified compounds 91.98% Oxygenated compounds 86.67 %

Hydrocarbons compounds 05.31 %

***RT:** Retention Time. ****RRT:** Relative Retention Time.

Table 3: Identified compounds of WFM from Head Space GC/MS.

No.	Name	RT*	RRT**	Base peak	Relative Area %	M. Weight	M. Formula
1	5,6-Epoxy-β-ionone	1.46	0.350	39	9.50	208	$C_{13}H_{20}O_2$
2	Nitrosamine	1.67	0.401	45	4.76	46	H_2N_2O
3	Acetone	1.73	0.415	43	0.56	58	C_3H_6O
4	Acetic acid	2.22	0.533	43	0.88	60	$C_2H_4O_2$
5	Hydroxyacetone (syn.: 1-Hydroxy-2-propanone)	2.83	0.680	43	0.43	74	$C_3H_6O_2$
6	3-Methyl-1-butanol (Fusel oil)	3.85	0.925	55	3.10	88	$C_5H_{12}O$
7	1,2-Propanediol	4.16	1.00	45	25.23	76	$C_3H_8O_2$
8	Butanoic acid	5.16	1.240	60	0.66	88	$C_4H_8O_2$
9	Ethyl butanoate (syn.: Ethyl butyrate)	5.30	1.274	71	0.87	116	$C_6H_{12}O_2$
10	Furfural			96	0.58	96	$C_5H_4O_2$
11	*Z*-3-Hexen-1-ol	6.79	1.632	41	1.23	100	$C_6H_{12}O$
12	α-Phellandrene	8.90	2.139	93	0.46	136	$C_{10}H_{16}$
13	α-Pinene	9.11	2.189	93	0.73	136	$C_{10}H_{16}$
14	β-Phellandrene	10.39	2.497	93	0.50	136	$C_{10}H_{16}$
15	β-Pinene	10.49	2.521	93	0.51	136	$C_{10}H_{16}$
16	Hexanoic acid	10.70	2.572	60	0.44	116	$C_6H_{12}O_2$
17	α-Terpinene	11.77	2.829	121	0.49	136	$C_{10}H_{16}$
18	Sylvestrene	12.17	2.925	93	0.58	136	$C_{10}H_{16}$
19	Benzyl alcohol	12.41	2..983	79	1.79	108	C_7H_8O
20	2,6-Dimethylhept-5-en-1-al	12.97	3.117	82	2.59	140	$C_9H_{16}O$
21	Isoamyl butyrate	13.12	3.153	71	3.46	158	$C_9H_{18}O_2$
22	Acetophenone	13.40	3.221	104	1.14	120	C_8H_8O
23	Menthol	16.76	4.028	71	1.35	156	$C_{10}H_{20}O$
24	Anethole	20.11	4.834	148	1.54	148	$C_{10}H_{12}O$
25	Benzyl butanoate	21.78	5.048	91	1.26	178	$C_{11}H_{14}O_2$
26	Vanillin	23.31	5.603	151	0.50	152	$C_8H_8O_3$
27	Cinnamyl isovalerate	30.27	7.276	85	3.46	218	$C_{14}H_{18}O_2$

Unidentified compounds 31.40 %

Identified compounds 68.60 %

Oxygenated compounds 60.57 %

Nitrogenous compounds 04.76 %

Hydrocarbons compounds 03.27 %

***RT:** Retention Time. ****RRT:** Relative Retention Time.

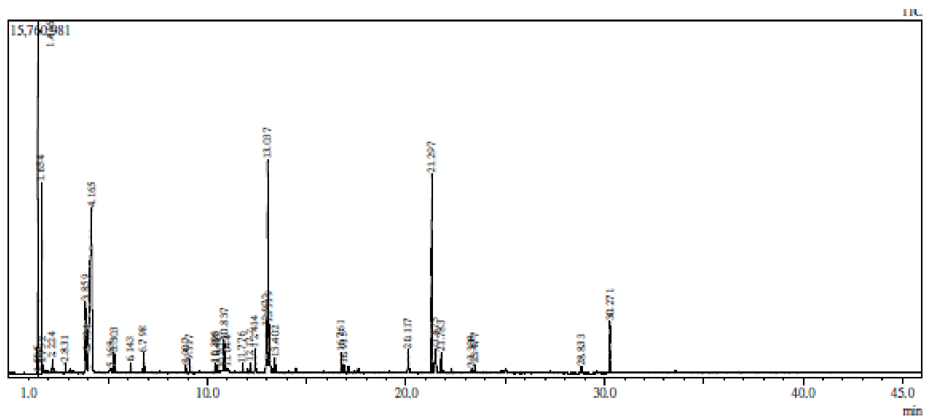

Figure 3: Total ion GC chromatogram of WFM.

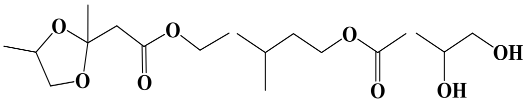

Figure 4: The major constituent for each sample.

5. Conclusion

The comparative study of Guava, Mixed Fruits and Watermelon Moâssel from Al Dandash Company (Egypt), exhibited relatively differences in the chemical constituents. Therefore, this study may introduce a toxicological effects prediction for these specimens.

6. Conflict of Interest

We declare that no conflict of interest.

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