

Utilizing SPME Arrow and GC-MS to Characterize the Aroma profile of Leading Seltzers Brands

2021 AOAC Annual Meeting

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1. Introduction

Whether it's a warm day at the beach or just a weekend afternoon spent at home, an alcoholic or hard seltzer is usually close by. The explosion of the hard seltzer segment has caught the attention of many companies eager to get in on the success. Early in 2018, only 10 hard seltzer brands were on the market. This increased to 26 brands by the beginning of 2019, and now more than 65 brands are fighting for consumers' attention and purchase.

But what sets the industry leading seltzers apart? In this study, two seltzer brands were analyzed via GC-MS. The headspace was sampled via SPME Arrow to extract the major fragrance and aroma inducing compounds. The analytes identified ranged from the major mono and sesquiterpenes to the additional ketones and ethylesters. By characterizing the headspace of several flavors including: cherry, lime, berry and grapefruit, aside by side comparison was created showing the individuality between the two brands.

Regardless of the flavor variety, compounds such as beta-myrcene, geraniol, D-limonene, linalool, isoamylacetate and ethylbutyrate were identified at varying concentrations. The use of SPME Arrow in addition to GCMS proves to be a useful advantage not only in the quality control of these beverages, but the R&D for new flavors or even the knowledge of competing flavor profiles.



Figure 1 Shimadzu GCMS-QP2020 NX with AOC-6000Plus Instrumental Conditions

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2. Experimental Approach

Two major seltzer brands were sampled via HS-SPME Arrow and analyzed on the QP2020 NX single quad. Across the two brands, nine unique flavors were run : black cherry, blueberry acai, grapefruit, lemon, lime, orange, raspberry lime, wild berry, and raspberry. Each of these flavors were run according to the parameters established in Table1.

For each flavor a TIC was acquired and was processed qualitatively in order to characterize the aroma profile from each beverage. Common terpenes and prominent volatile compounds usually found in beverages were identified. A chromatogram for Lemon Seltzer 1 can be found below in Figure 2. The corresponding compounds of interest and their area counts were collated into Table2.

After all flavors were characterized, three common flavors between two brands were compared qualitatively: lime, grapefruit, and black cherry. The chromatograms were overlaid to distinguish the chromatography and overall display the differences in peak area and height.

Instrumental Conditions

Table 1 Analytical conditions

GC		MS	
Inlet	250C	Transfer Line	250C
Column	Stabilwax-MS	Ion source	200C
Carrier Gas	Helium	Scan	40-500 m/z
Linear velocity	41.3 cm/s		
Split ratio	20		
AOC -6000Plus			
SPME Arrow	DVB/CAR/PDMS	Incubation Time	10min
Incubation Temp	60C	Sampling time	10min

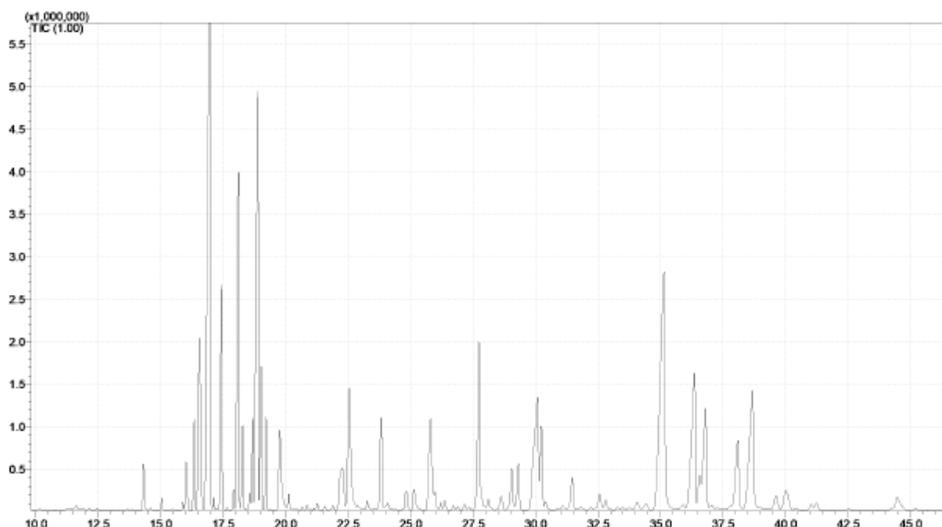


Figure 2 Chromatogram for Lemon seltzer 1

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Table 2 Compound table for Lemon Seltzer 1

Compound	RT	Area	Height	SI
Ethyl Acetate	5.501	608719	129869	99
Ethanol	7.085	15065536	1219638	99
Ethyl Butyrate	11.622	48547	9677	98
Camphene	12.46	15655	3592	97
Isobutanol	14.586	68133	11900	97
Isoamyl acetate	15.035	179410	48585	99
.beta.-Myrcene	16.011	648210	135541	100
D-Limonene	16.96	8275299	1057102	99
Eucalyptol	17.436	1172227	297366	100
.gamma.-Terpinene	18.102	4578834	937079	100
Acetic acid, hexyl ester	19.217	1239481	340769	100
Octanal	19.764	788478	113458	100
Linalool	20.124	79812	28363	99
Sulcatone	21.263	56211	17322	98
Nonanal	22.546	1451799	168746	99
Acetic acid	25.127	593169	83530	99
Decanal	25.799	913491	95016	100
(+)-2-Bornanone	26.878	30265	5581	97
Benzaldehyde	27.331	42307	7104	96
Linalool	27.732	1656491	283383	99
1-Octanol	28.096	77701	14376	96
Fenchol	29.304	531096	91238	100
Propylene Glycol	30.076	10420485	931807	97
.alpha.-Cyclogeraniol acetate	31.799	43475	7245	95
Isoborneol	33.261	54109	7581	97
trans-Ocimenol	33.734	13957	2257	86
.alpha.-Terpineol	35.123	5430672	425966	99
(-)-Carvone	37.047	87010	11569	95
.alpha.-Terpinyl acetate	37.323	16441	2390	95
Geranyl acetate	38.67	3636766	330716	100
Citronellol	38.952	22276	3410	94
Geraniol	44.463	392819	40038	98
Phenylethyl Alcohol	49.206	439799	34510	99
Caryophyllenyl alcohol	59.007	47683	7474	98

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3. Result

SPME Arrow was extremely effective at recovering several prominent terpenes and aromatics from the lemon seltzer. Limonene and linalool have a clear presence as expected as well as geraniol. Some unexpected detections appeared later in the run with fenchol and caryophyllenyl alcohol. Below are the comparison TICs of seltzer1 (black) and seltzer2 (pink). Figure 3, 4, and 5 show the TICs for grapefruit, black cherry, and lime respectively. Base shift was applied to highlight differences in the chromatograms.

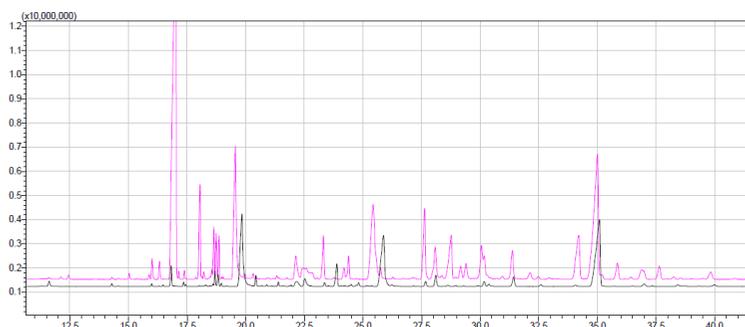


Figure 3 Chromatogram for Grapefruit

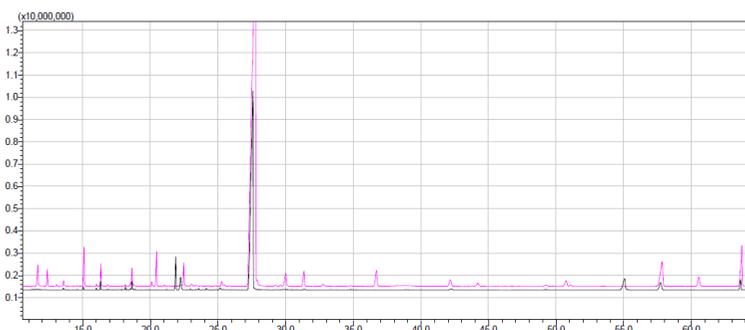


Figure 4 Chromatogram for Black cherry

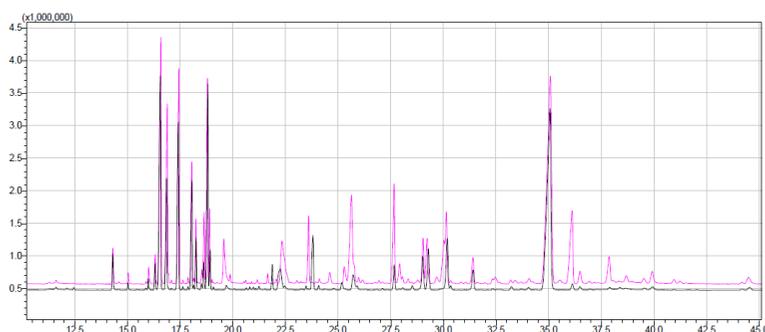


Figure 5 Chromatogram for Lime

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4. Conclusion

HS-SPME Arrow paired with GCMS proves more than efficient for the characterization of the headspace and aroma profiles of seltzers. The detection of several expected terpenes and additional volatiles that have an affect on taste and aroma, is easily obtainable. The methodology used here also proved useful in comparing multiple brands of seltzers unlocking the potential for quality control and quality assurance capabilities. Further quantitative work is expected to determine overall linearity and effectiveness of the method.

First Edition: September, 2021