Application Note

Instrument: Pegasus® BT GC-TOFMS

Raw Material Screening with GC-MS: Flavor Analysis of Malted Grain from Hot Steeped Malt

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Key Words:GC-MS, GC-TOFMS, Pegasus BT, HS-SPME, Raw Materials, Malted Barley

Introduction

The ability to screen raw ingredients early in the production process for a food or beverage is useful for quality control, and also for identifying process modifications or optimizations to achieve the desired characteristics of the product. For beer, malted barley is one of the primary ingredients and it is added early in the brewing process. It provides complex carbohydrates and sugars that are crucial for fermentation and it also imparts flavor, body, and color to the final product. The flavor contribution depends largely on the style of malt used. Base, caramel, and dark roasted malts are all common and each lends unique flavor notes and characteristics. Traditionally, a chew test of whole kernels has been used as a check for flavor and freshness. While this test provides insight and has the benefit of being very fast, it does not fully reflect the flavors that are extracted during the brewing process that would be anticipated in the final product. The American Society of Brewing Chemists has a published Method of Analysis, the "Hot Steep Malt Sensory Evaluation Method",[1] to prepare malt extracts for sensory analysis that are more representative of the malt in the beer. Chemical analyses are good complements to traditional sensory analysis and here we aim to further investigate these types of samples with a non-targeted chemical analysis. Head space solid phase micro-extraction (HS-SPME) was used to collect the volatile and semi-volatile flavor analytes, and gas chromatography coupled to mass spectrometry (GC-MS) was used for subsequent analysis. A variety of malt extracts were prepared and analyzed yielding data that provided information on individual analytes differentiating these malt styles. Many of the observed analytes have known flavor and odor properties which can be connected with the sensory attributes of the malts.

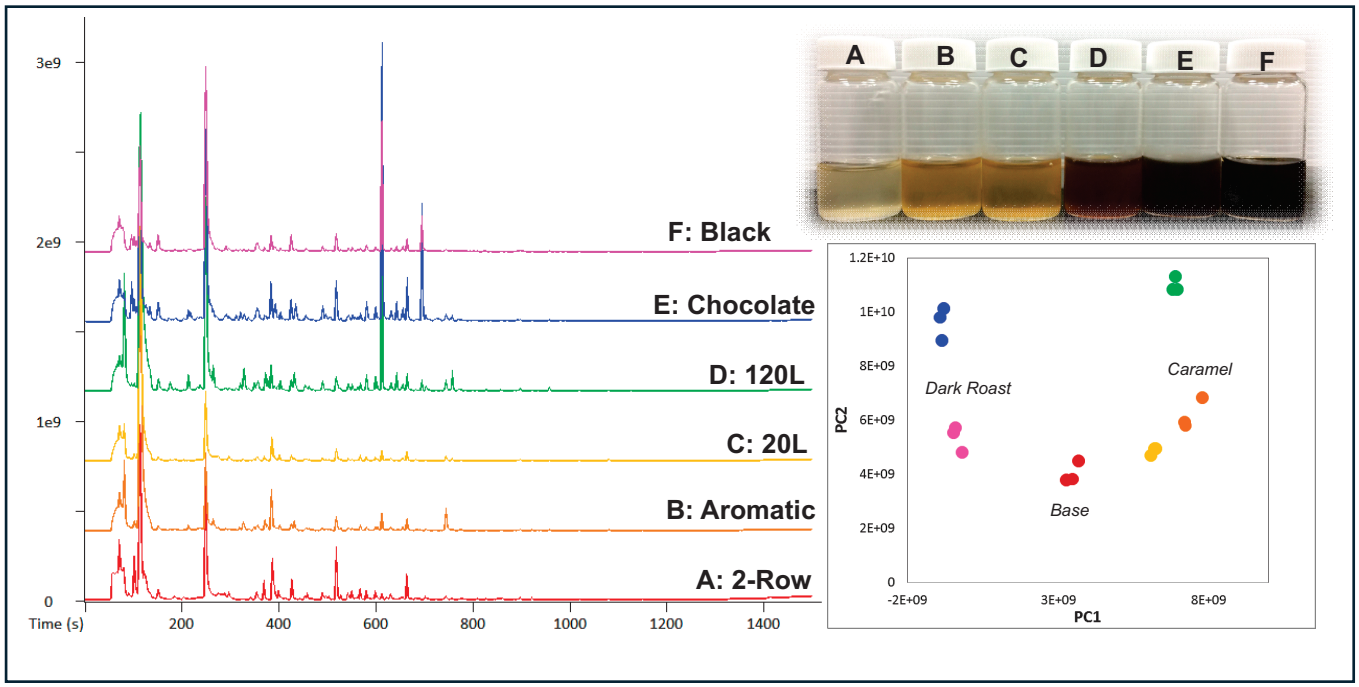


Figure 1. Six malt extracts were compared. Representative Total Ion chromatograms (TIC) and pictures are shown for each and PCA of the TIC traces was performed.

Experimental

Six varieties of malted barley, listed in Table 1, were prepared for analysis based on the ASBC's "Hot Steep Malt Sensory Evaluation Method."[1] For this work, the method was scaled to 20% due to the reduced volume required for analytical analysis compared to sensory analysis. For each malt variety, 10 g of ground malt were added to 80 mL of 65 °C water in an insulated thermos and mixed with shaking. After 15 minutes of extraction, the contents were swirled and filtered, resulting in the malt extract/wort samples. As advised in the protocol, base malts were analyzed at 100%, specialty malts were mixed with base malt at 50%, and dark roasted specialty malts were mixed with base malt at 15%. For each sample, 5 mL of wort were pipet into a 20 mL glass vial with septum cap. The samples were incubated for 5 min at 35 °C and then extracted with a DVB/CAR/PDMS fiber (Supelco) for 10 min at the same temperature. Each sample was then analyzed by GC-MS with the Pegasus BT (LECO). All analytical data for a given sample was acquired within 4 h of filtration. Instrument conditions are listed in Table 2.

Table 1. Malted Barley Varieties

Sample	Name	Malt Type	Inclusion Level	Lovibond
A	2-Row	Base	100 %	1.8
B	Aromatic	Specialty	50 %	20
C	Caramel 20L	Specialty	50 %	20
D	Caramel 120L	Specialty	50 %	120
E	Chocolate	Dark Roast Specialty	15 %	350
F	Black	Dark Roast Specialty	15 %	500

Table 2. GC-TOFMS (Pegasus BT) Conditions

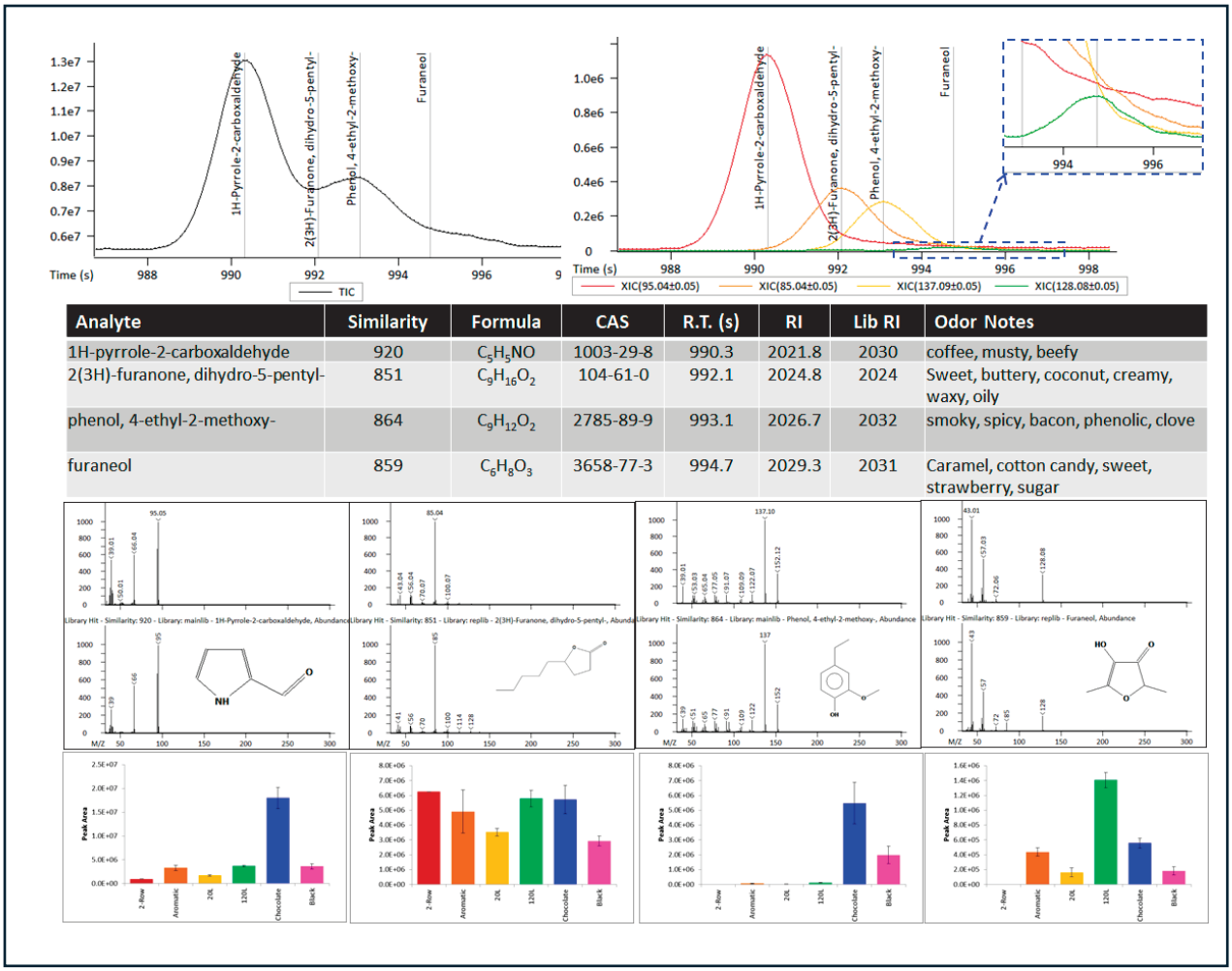
Gas Chromatograph	**Agilent 7890 with LECO L-PAL 3 Autosampler**
Injection	SPME, 3 min desorption in 250 °C inlet
Carrier Gas	He @ 1.4 mL/min, Constant Flow
Column One	Stabilwax, 30 m x 0.25 mm i.d. x 0.25 μm coating (Restek)
Temperature Program	3 min at 40 °C, ramped 10 °C/min to 250 °C, hold 1 min
Transfer Line	250 °C with uncoated guard column
Mass Spectrometer	**LECO *Pegasus* BT**
Ion Source Temperature	250 °C
Mass Range	33-500 m/z
Acquisition Rate	10 spectra/s

Results and Discussion

Different malt styles are produced by altering the temperature and duration of kiln heating and/or roasting of the barley. These conditions drive various reactions, and alterations will yield a range of malt styles and impact the types and amounts of the reaction by-products produced. Both caramelization, the breakdown of sugars, and the Maillard reaction, the reaction of a reducing sugar with an amino acid, are anticipated and have by-products with important odor and flavor characteristics. The malt styles are categorized as base, specialty, or dark roast specialty with the darker roasted malts generally heated to higher temperatures for greater lengths of time. Extracts from six varieties of malted barley, shown in Figure 1 and described in Table 1, were analyzed and compared. These included a base malt, three specialty malts, and two dark roast specialty malts. Chromatograms for each of the extracts, shown in Figure 1, represent the aroma profiles of each sample. Some similarities and many differences are apparent between the samples and preliminary general characterization was done with Principle Component Analysis (PCA) of the TIC traces. The scores plot, where each sample is represented as a data point, is shown in Figure 1. The extracts from each malted barley variety distinctly cluster and the dark specialty roast samples have lower PC1 scores while the caramel malts have higher PC1 scores.

The general distinction of these samples can be further explored by looking at trends of individual analytes across the malt varieties. With this analytical technique, individual analytes are separated from each other both chromatographically and mathematically. Chromatographic coelution still frequently occurs with complex samples and many of these cases can be distinguished with mathematical deconvolution of the full mass range TOFMS data, as demonstrated in Figure 2. There are two apparent peaks in the TIC, but spectral patterns indicate the coelution of four analytes. By plotting masses unique to each, the peak shapes can be observed and integrated to provide peak areas and information on the relative trend across the samples. Pure spectral information for each analyte is also generated and when matched with commercially available libraries, provides tentative identification information from which odor characteristics can be determined. These four analytes, that were confounded in the TIC, have interesting odor characteristics and distinctly different trends that were observed because of deconvolution capabilities. 2(3H)-furanone, dihydro-5-pentyl is observed in all of the samples with only subtle differences between the malt styles. This analyte has sweet, buttery, coconut, creamy, waxy, and oily odor descriptors. Furaneol has caramel, cotton candy, sweet, strawberry, and sugar odor descriptors and is observed at highest levels in the 120L caramel malt with varying levels in the other styles. 1H-pyrrole-2-carboxaldehyde and 4-ethyl-2-methoxy phenol were both observed at highest levels in the chocolate malt. The pyrrole has coffee and musty odor descriptors while the phenol has odor descriptors of

smoky, spicy, bacon, phenolic, and clove. The decrease in the levels in the black malt is potentially attributed to thermal breakdown as black malt is often heated to higher temperatures (above 260 °C), driving further reactions and also surpassing the boiling point of some of these compounds (217-219 °C and 234-236 °C for the pyrrole and phenol compounds, respectively).



Analyte	Similarity	Formula	CAS	R.T. (s)	RI	Lib RI	Odor Notes
1H-pyrrole-2-carboxaldehyde	920	C_5H_5NO	1003-29-8	990.3	2021.8	2030	coffee, musty, beefy
2(3H)-furanone, dihydro-5-pentyl-	851	$C_9H_{16}O_2$	104-61-0	992.1	2024.8	2024	Sweet, buttery, coconut, creamy, waxy, oily
phenol, 4-ethyl-2-methoxy-	864	$C_9H_{12}O_2$	2785-89-9	993.1	2026.7	2032	smoky, spicy, bacon, phenolic, clove
furaneol	859	$C_6H_8O_3$	3658-77-3	994.7	2029.3	2031	Caramel, cotton candy, sweet, strawberry, sugar

Figure 2. Deconvolution separates four individual analytes that appear as two peaks in the TIC. These analytes are present at different levels in each sample, likely contributing to some of the flavor differences related to malt variety used.

Many other individual analytes were observed and information for nearly 200 compounds was compiled in Figure 3 and Appendix A. These specific analytes were identified based on mass spectral similarity (>800) compared to the NIST 2017 database and retention index matching (library vs observed < 40 RI units). A wide range of analyte types were observed, including: alcohols, aldehydes, ketones, hydrocarbons, aromatics, esters, furans, pyranones, pyrazines, pyridines, pyrroles, sulfides, thiophenes, etc. Information on these tentative analyte identifications is compiled in Appendix A. Relative peak area trends were also determined across the malted barley varieties, demonstrated in the heat map, with several distinct trends observed.

A collection of specific analytes are highlighted in Figure 4 with additional details compiled. These analytes may be of particular interest because of their known relationships to malting and/or brewing. Dimethyl sulfide (DMS) is produced during germination and the early stages of kilning, and is an important odor compound with sulfury or corn descriptors. As a volatile compound, it can be driven off during the higher temperature kilning or roasting of specialty and dark specialty roasted malts. As expected, DMS was observed at highest levels in the base malt and at lower levels in the specialty and dark roast specialty malts. Methional is also an important odor compound related to beer and has potato odor characteristics. This is a breakdown product of the amino acid, methionine, and is often a target of routine screening. We observe methional at highest levels in the Aromatic and Caramel 120L malts. By-products of carmelization and the Maillard reaction are also anticipated and nitrogen-containing rings, like 2-6-dimethyl pyrazine, are potential Maillard reaction products while maltol is likely a caramelization product. The trends of these specific analytes and other similar analytes across the 120L, Chocolate, and Black malts may shed light on the types of reactions occurring for each type of malt.

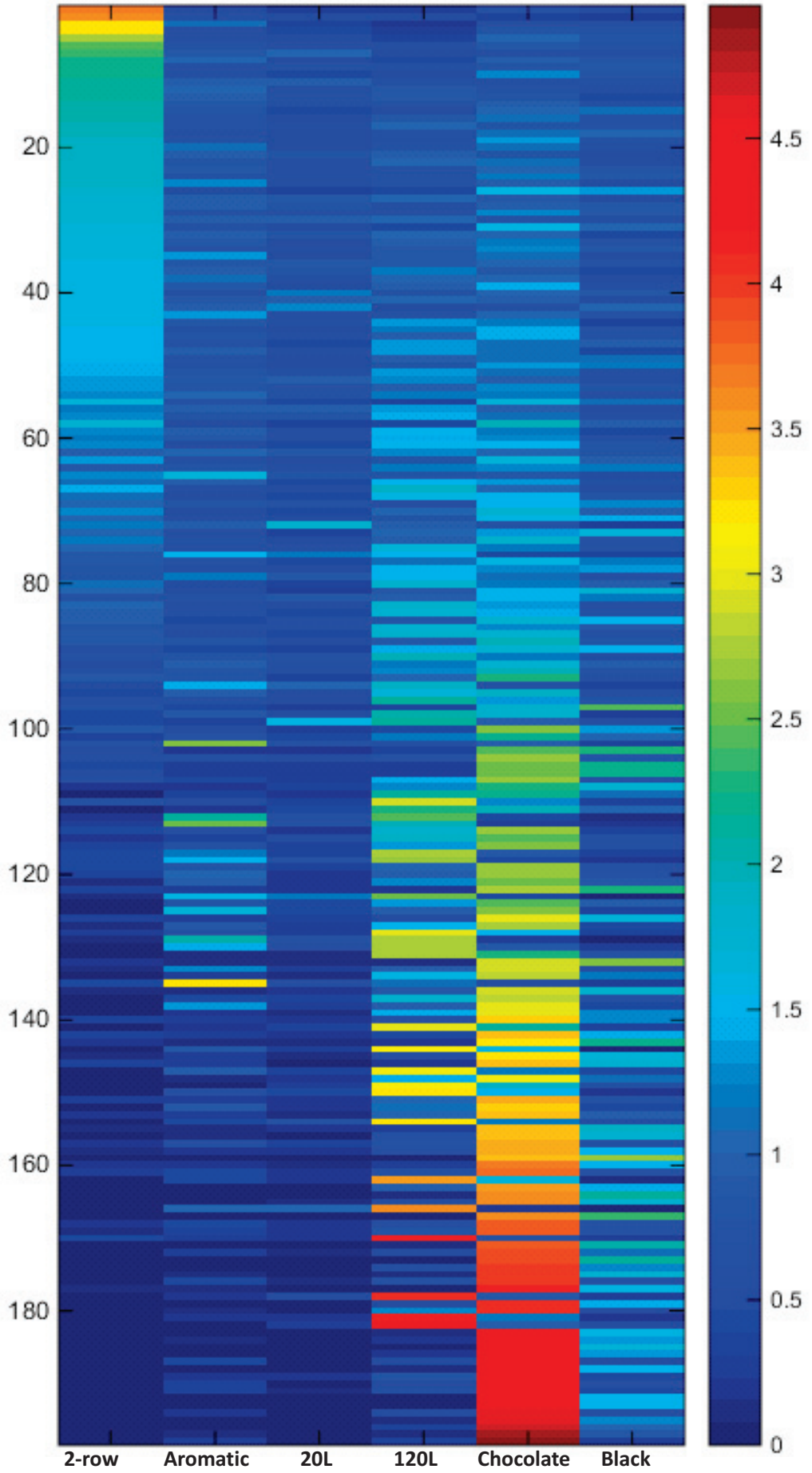


Figure 3. Peak area trends by malt variety.

Analyte	Similarity	Formula	CAS	R.T. (s)	RI	Lib RI	Odor Notes
dimethyl sulfide	976	C_2H_6S	75-18-3	70.5	794	754	sulfury, onion, sweet, corn, vegetable, cabbage, tomato, green radish
methional	887	C_4H_8OS	3268-49-3	603.2	1453.2	1454	musty, potato, tomato, earthy, vegetable, creamy
2,6-dimethyl-pyrazine	882	$C_6H_8N_2$	108-50-9	490.7	1320.3	1328	cocoa, roasted, nuts, roast beef, coffee
maltol	916	$C_6H_6O_3$	118-71-8	955.9	1964.4	1969	sweet, caramel, cotton candy, jam, fruity, baked bread

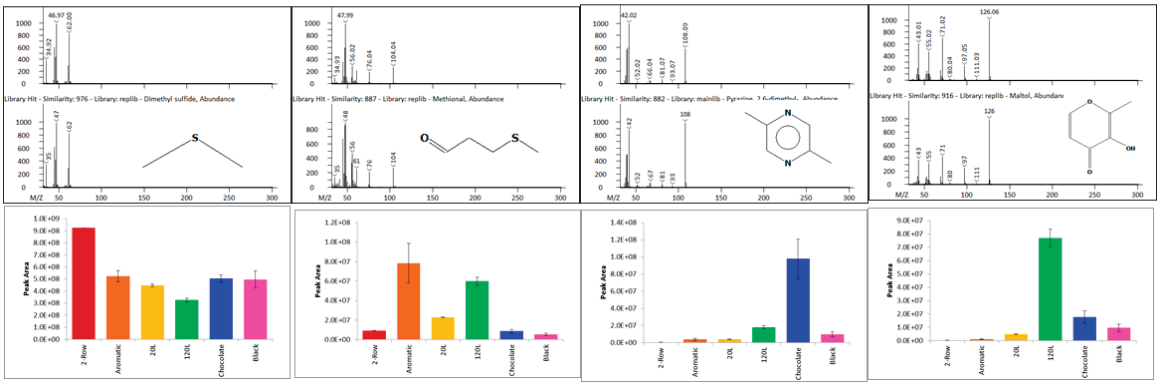


Figure 4. Representative analytes with distinct trends related to the malt varieties are shown.

Conclusion

In this work, we demonstrate an analytical method for analyzing malt extracts, prepared by the ASBC's "Hot Steep Malt Sensory Evaluation Method" intended for sensory analysis. The malt extracts were sampled with HS-SPME and analyzed with GC-MS. This analytical approach can provide good complementary data on individual analytes and help uncover more about your sample. Hundreds of analytes were identified and compared, with many malt specific trends observed. Many caramelization and Maillard reaction products were observed at elevated levels in the samples roasted at higher temperatures.

References

[1]"Hot Steep Malt Sensory Evaluation Method," Sensory Analysis – 14, ASBC Methods of Analysis.

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Appendix

Tentative identifications of analytes shown in Figure 3.

#	Name	CAS	Similarity	R.T. (s)	RI	Lib RI	Formula
1	pentane, 1-chloro-	543-59-9	872	125.2	939.9	945	$C_5H_{11}Cl$
2	methylene chloride	75-09-2	939	121.4	933.6	933	CH_2Cl_2
3	trichloromethane	67-66-3	913	188.7	1025.3	1022	$CHCl_3$
4	ethyl acetate	141-78-6	948	101.2	900.2	888	$C_4H_8O_2$
5	propanoic acid, 2-methyl-, ethyl ester	97-62-1	873	141.4	966.7	961	$C_6H_{12}O_2$
6	acetoin	513-86-0	874	458.4	1285	1284	$C_4H_8O_2$
7	m-cymene	535-77-3	817	436.6	1262.5	1269	$C_{10}H_{14}$
8	butanoic acid, 3-methyl-, ethyl ester	108-64-5	875	235.0	1068.4	1068	$C_7H_{14}O_2$
9	hexanoic acid, ethyl ester	123-66-0	909	405.0	1229.9	1233	$C_8H_{16}O_2$
10	propanoic acid, 2-hydroxy- ethyl ester	97-64-3	949	509.7	1342.1	1347	$C_5H_{10}O_3$
11	pseudocumene	95-63-6	804	444.5	1270.7	1283	C_9H_{12}
12	ethanol	64-17-5	931	121.9	934.5	932	C_2H_6O
13	decanoic acid, ethyl ester	110-38-3	877	739.8	1634.4	1638	$C_{12}H_{24}O_2$
14	methane, tribromo-	75-25-2	810	592.0	1439.4	1430	$CHBr_3$
15	butanoic acid, 2-methyl-, ethyl ester	7452-79-1	890	218.4	1052.9	1051	$C_7H_{14}O_2$
16	3-hexen-1-ol	544-12-7	850	544.8	1382.2	1391	$C_6H_{12}O$
17	1-penten-3-one	1629-58-9	906	187.0	1023.7	1019	C_5H_8O
18	acetic acid, hexyl ester	142-92-7	918	443.1	1269.2	1272	$C_8H_{16}O_2$
19	1-hexanol	111-27-3	951	517.9	1351.4	1355	$C_6H_{14}O$
20	pyrazine, 2-methoxy-3-(1-methylpropyl)-	24168-70-5	813	637.2	1495.6	1500	$C_9H_{14}N_2O$
21	dodecanoic acid, ethyl ester	106-33-2	837	876.8	1837.4	1841	$C_{14}H_{28}O_2$
22	acetic acid, 2-phenylethyl ester	103-45-7	922	860.2	1811.3	1813	$C_{10}H_{12}O_2$
23	2-nonanone	821-55-6	817	545.5	1383	1390	$C_9H_{18}O$
24	2-hexenal	505-57-7	936	390.0	1214.4	1213	$C_6H_{10}O$
25	phenylethyl alcohol	60-12-8	918	921.6	1908.2	1906	$C_8H_{10}O$
26	toluene	108-88-3	943	203.5	1039.1	1042	C_7H_8
27	2,4-di-tert-butylphenol	96-76-4	903	1150.1	2308.8	2318	$C_{14}H_{22}O$
28	dimethyl sulfide	75-18-3	979	70.5	794	754	C_2H_6S
29	1-penten-3-ol	616-25-1	876	339.6	1166	1159	$C_5H_{10}O$
30	n-decanoic acid	334-48-5	902	1137.1	2284.2	2276	$C_{10}H_{20}O_2$
31	decane	124-18-5	839	164.1	1002.4	1000	$C_{10}H_{22}$
32	5,9-undecadien-2-one, 6,10-dimethyl-(E)-	3796-70-1	847	884.4	1849.2	1859	$C_{13}H_{22}O$
33	1-heptanol	111-70-6	906	602.4	1452.3	1453	$C_7H_{16}O$
34	2-octanone	111-13-7	941	453.1	1279.5	1287	$C_8H_{16}O$
35	benzeneacetic acid, ethyl ester	101-97-3	892	841.2	1782.3	1783	$C_{10}H_{12}O_2$
36	naphthalene	91-20-3	858	809.5	1734.9	1745	$C_{10}H_8$
37	5-ethylcyclopent-1-enecarboxaldehyde	36431-60-4	849	567.8	1409.3	1410	$C_8H_{12}O$
38	octanoic acid, ethyl ester	106-32-1	875	586.9	1433	1435	$C_{10}H_{20}O_2$
39	5-hepten-2-one, 6-methyl-	110-93-0	904	502.8	1334.2	1338	$C_8H_{14}O$
40	butanenitrile, 3-methyl-	625-28-5	942	296.5	1125.7	1125	C_5H_9N
41	octanoic acid	124-07-2	884	1020.1	2072.9	2060	$C_8H_{16}O_2$
42	limonene	138-86-3	834	360.4	1185.4	1200	$C_{10}H_{16}$
43	1-propanol, 2-methyl-	78-83-1	933	271.0	1102	1092	$C_4H_{10}O$
44	linalool	78-70-6	848	673.9	1544.3	1547	$C_{10}H_{18}O$
45	3,5-octadien-2-one	38284-27-4	864	652.9	1516.3	1522	$C_8H_{12}O$
46	2,6-nonadienal, (E,Z)-	557-48-2	933	701.7	1581.5	1584	$C_9H_{14}O$
47	nonanal	124-19-6	931	550.5	1388.7	1391	$C_9H_{18}O$
48	1-hexanol, 2-ethyl-	104-76-7	957	630.4	1487.1	1491	$C_8H_{18}O$
49	2(3H)-furanone, 5-ethyldihydro-	695-06-7	924	785.0	1698.2	1694	$C_6H_{10}O_2$
50	1-pentanol	71-41-0	957	424.6	1250.1	1250	$C_5H_{12}O$
51	1-octanol	111-87-5	868	681.6	1554.7	1557	$C_8H_{18}O$
52	furan, 2-pentyl-	3777-69-3	952	400.7	1225.4	1231	$C_9H_{14}O$
53	2-pentenal, (E)-	1576-87-0	819	299.8	1128.9	1127	C_5H_8O
54	2(3H)-furanone, dihydro-5-pentyl-	104-61-0	877	992.1	2024.8	2024	$C_9H_{16}O_2$
55	3-pentanone, 2-methyl-	565-69-5	888	163.0	1001.3	1003	$C_6H_{12}O$
56	acetic acid	64-19-7	936	620.2	1474.4	1449	$C_2H_4O_2$
57	2-octen-1-ol, (E)-	18409-17-1	901	724.0	1612.1	1614	$C_8H_{16}O$
58	isobutyl acetate	110-19-0	839	179.6	1016.8	1012	$C_6H_{12}O_2$
59	benzophenone	119-61-9	922	1234.0	2473.7	2450	$C_{13}H_{10}O$
60	3,5-octadien-2-one, (E,E)-	30086-02-3	905	690.6	1566.7	1570	$C_8H_{12}O$
61	2,4-heptadienal, (E,E)-	4313-03-5	821	632.3	1489.5	1495	$C_7H_{10}O$
62	o-xylene	95-47-6	832	350.0	1175.7	1186	C_8H_{10}
63	1-butanol, 3-methyl-, acetate	123-92-2	897	288.9	1118.7	1122	$C_7H_{14}O_2$
64	heptanal	111-71-7	814	354.2	1179.6	1184	$C_7H_{14}O$
65	1-butanol, 3-methyl-	123-51-3	952	384.3	1208.5	1209	$C_5H_{12}O$
66	2-butenal	4170-30-3	839	207.1	1042.4	1047	C_4H_6O
67	2,4-decadienal, (E,Z)-	25152-83-4	883	827.1	1761.1	1754	$C_{10}H_{16}O$
68	2-heptenal, (E)-	18829-55-5	904	489.7	1319.2	1323	$C_7H_{12}O$
69	p-xylene	106-42-3	888	302.7	1131.6	1138	C_8H_{10}
70	2,3-butanedione (diacetyl)	431-03-8	870	152.0	984.2	979	$C_4H_6O_2$
71	acetone	67-64-1	926	82.1	834.2	819	C_3H_6O
72	nonanoic acid	112-05-0	920	1079.6	2178.2	2171	$C_9H_{18}O_2$
73	pentanal	110-62-3	930	150.4	981.6	979	$C_5H_{10}O$
74	2-nonenal, (E)-	18829-56-6	961	664.1	1531.2	1534	$C_9H_{16}O$
75	2-n-butyl furan	4466-24-4	834	297.6	1126.8	1123	$C_8H_{12}O$

#	Name	CAS	Similarity	R.T. (s)	RI	Lib RI	Formula
76	butanal, 3-methyl-	590-86-3	910	113.8	921	918	$C_5H_{10}O$
77	2-heptanone	110-43-0	934	353.8	1179.2	1182	$C_7H_{14}O$
78	hexanal	66-25-1	957	249.1	1081.6	1083	$C_6H_{12}O$
79	butanoic acid, 3-methyl-	503-74-2	884	774.9	1684	1666	$C_5H_{10}O_2$
80	3-octen-2-one	1669-44-9	846	561.5	1401.4	1411	$C_8H_{14}O$
81	acetic acid, pentyl ester	628-63-7	915	346.0	1171.9	1176	$C_7H_{14}O_2$
82	styrene	100-42-5	902	427.0	1252.6	1260	C_8H_8
83	1-octen-3-ol	3391-86-4	914	599.0	1448.1	1450	$C_8H_{16}O$
84	2,4-nonadienal, (E,E)-	5910-87-2	872	784.1	1697	1700	$C_9H_{14}O$
85	furan, 2-ethyl-	3208-16-0	897	133.3	953.3	950	C_6H_8O
86	hexanoic acid	142-62-1	942	891.5	1860.5	1846	$C_6H_{12}O_2$
87	2-octenal, (E)-	2548-87-0	947	580.3	1424.8	1429	$C_8H_{14}O$
88	benzyl alcohol	100-51-6	847	899.9	1873.6	1870	C_7H_8O
89	butyrolactone	96-48-0	941	733.8	1625.9	1632	$C_4H_6O_2$
90	cyclohexanone, 2,2,6-trimethyl-	2408-37-9	881	477.1	1304.8	1319	$C_9H_{16}O$
91	benzaldehyde	100-52-7	957	655.4	1519.6	1520	C_7H_6O
92	benzaldehyde, 4-ethyl-	4748-78-1	837	788.5	1703.5	1721	$C_9H_{10}O$
93	pyrrole	109-97-7	895	652.2	1515.3	1514	C_4H_5N
94	butanal, 2-methyl-	96-17-3	915	111.5	917.2	914	$C_5H_{10}O$
95	2-heptanone, 6-methyl-	928-68-7	900	409.7	1234.7	1237	$C_8H_{16}O$
96	octanal	124-13-0	864	458.3	1285	1289	$C_8H_{16}O$
97	4-heptenal, (Z)-	6728-31-0	903	413.9	1239.1	1240	$C_7H_{12}O$
98	2-methoxy-4-vinylphenol	7786-61-0	830	1088.1	2193.3	2188	$C_9H_{10}O_2$
99	benzonitrile	100-47-0	877	716.7	1601.7	1589	C_7H_5N
100	acetic acid, methyl ester	79-20-9	959	84.1	841.2	828	$C_3H_6O_2$
101	indole	120-72-9	856	1218.3	2442.2	2445	C_8H_7N
102	thiophene, 3-phenyl-	2404-87-7	855	1052.3	2129.4	2116	$C_{10}H_8S$
103	2-butanone	78-93-3	937	106.2	908.4	907	C_4H_8O
104	acetophenone	98-86-2	871	748.7	1646.9	1647	C_8H_8O
105	pyridine, 2-ethyl-	100-71-0	897	448.4	1274.7	1278	C_7H_9N
106	ethylbenzene	100-41-4	903	287.9	1117.7	1129	C_8H_{10}
107	2(3H)-furanone, 5-methyl-	591-12-8	805	584.5	1430.1	1426	$C_5H_6O_2$
108	2,5-furan dicarboxaldehyde	823-82-5	912	965.5	1980.2	1991	$C_6H_4O_3$
109	2-cyclopenten-1-one, 2-hydroxy-3-methyl-	80-71-7	820	868.5	1824.3	1830	$C_6H_8O_2$
110	2,4-decadienal, (E,E)-	25152-84-5	845	856.6	1805.5	1811	$C_{10}H_{16}O$
111	5-hydroxymethylfurfural	67-47-0	857	1246.7	2499.4	2496	$C_6H_6O_3$
112	benzeneacetaldehyde, α-ethylidene-	4411-89-6	895	933.8	1928.1	1929	$C_{10}H_{10}O$
113	methional	3268-49-3	899	603.2	1453.2	1454	C_4H_8OS
114	maleic anhydride	108-31-6	803	563.9	1404.4	1420	$C_4H_2O_3$
115	2-propanone, 1-hydroxy-	116-09-6	919	471.0	1298.1	1303	$C_3H_6O_2$
116	2-butenal, 2-methyl-	1115-11-3	824	260.5	1092.2	1095	C_5H_8O
117	2-pentenal, 2-methyl-	623-36-9	806	329.9	1157	1155	$C_6H_{10}O$
118	propanal, 2-methyl-	78-84-2	954	80.6	829.2	819	C_4H_8O
119	pyrazine, trimethyl-	14667-55-1	874	555.8	1394.8	1402	$C_7H_{10}N_2$
120	1H-pyrrole-2-carboxaldehyde, 1-ethyl-	2167-14-8	809	719.1	1605.1	1610	C_7H_9NO
121	4,5-dimethyl-2-isobutyloxazole	26131-91-9	836	505.6	1337.3	1330	$C_9H_{15}NO$
122	benzene, propyl-	103-65-1	892	375.5	1199.5	1212	C_9H_{12}
123	5-methyl-2-phenyl-2-hexenal	21834-92-4	873	1018.9	2070.8	2056	$C_{13}H_{16}O$
124	ethanone, 1-(2-pyridinyl)-	1122-62-9	843	713.7	1597.6	1597	C_7H_7NO
125	pyrazine, 2,5-dimethyl-3-(3-methylbutyl)-	18433-98-2	873	750.2	1649	1666	$C_{11}H_{18}N_2$
126	phenol	108-95-2	937	980.9	2005.6	2000	C_6H_6O
127	pyrazine, 2,5-dimethyl-	123-32-0	902	485.2	1314.1	1320	$C_6H_8N_2$
128	2,3-pentanedione	600-14-6	939	231.1	1064.8	1058	$C_5H_8O_2$
129	benzeneacetaldehyde, α-(2-ethylpropylidene)-	26643-91-4	831	939.7	1937.8	1926	$C_{12}H_{14}O$
130	ethanone, 1-(1H-pyrrol-2-yl)-	1072-83-9	925	957.9	1967.7	1973	C_6H_7NO
131	ethanone, 1-(2-furanyl)-	1192-62-7	945	642.6	1502.5	1499	$C_6H_6O_2$
132	benzene, n-butyl-	104-51-8	931	476.7	1304.3	1312	$C_{10}H_{14}$
133	pyrazine, 3-ethyl-2,5-dimethyl-	13360-65-1	914	589.9	1436.7	1443	$C_8H_{12}N_2$
134	ethanone, 1-(1-methyl-1H-pyrrol-2-yl)-	932-16-1	867	751.6	1651.1	1656	C_7H_9NO
135	benzeneacetaldehyde	122-78-1	935	744.3	1640.7	1640	C_8H_8O
136	furan	110-00-9	923	77.6	818.8	798	C_4H_4O
137	3(2H)-furanone, dihydro-2-methyl-	3188-00-9	866	435.9	1261.8	1268	$C_5H_8O_2$
138	pyrazine, 2,5-dimethyl-3-(2-methylpropyl)-	32736-94-0	803	653.6	1517.2	1520	$C_{10}H_{16}N_2$
139	furfural	98-01-1	965	612.0	1464.2	1462	$C_5H_4O_2$
140	methyl isobutyl ketone	108-10-1	908	172.3	1010	1010	$C_6H_{12}O$
141	2-vinylfuran	1487-18-9	871	242.8	1075.7	1063	C_6H_6O
142	thiophene	110-02-1	940	187.6	1024.3	1025	C_4H_4S
143	m-cresol	108-39-4	845	1029.6	2089.1	2091	C_7H_8O
144	disulfide, dimethyl	624-92-0	924	236.8	1070.1	1077	$C_2H_6S_2$
145	pyridine	110-86-1	958	351.2	1176.8	1185	C_5H_5N
146	2-cyclopenten-1-one, 2-methyl-	1120-73-6	861	527.4	1362.3	1367	C_6H_8O
147	furaneol	3658-77-3	859	994.7	2029.3	2031	$C_6H_8O_3$
148	2(5H)-furanone	497-23-4	928	821.5	1752.8	1742	$C_4H_4O_2$
149	2-furanmethanol, acetate	623-17-6	885	667.5	1535.7	1531	$C_7H_8O_3$
150	furan, 3-phenyl-	13679-41-9	896	885.5	1851	1849	$C_{10}H_8O$
151	benzaldehyde, 2-methyl-	529-20-4	891	729.3	1619.5	1632	C_8H_8O
152	pyrazine, 2-ethyl-5-methyl-	13360-64-0	820	545.5	1383	1387	$C_7H_{10}N_2$

#	Name	CAS	Similarity	R.T. (s)	RI	Lib RI	Formula
153	oxazole, trimethyl-	20662-84-4	901	365.1	1189.8	1197	C_6H_9NO
154	2-furanmethanol, 5-methyl-	3857-25-8	859	799.3	1719.6	1714	$C_6H_8O_2$
155	thiophene, 2-methyl-	554-14-3	864	255.0	1087.1	1097	C_5H_6S
156	2-propanone, 1-(acetyloxy)-	592-20-1	934	613.7	1466.3	1474	$C_5H_8O_3$
157	1H-pyrrole-2-carboxaldehyde	1003-29-8	925	990.3	2021.8	2030	C_5H_5NO
158	p-cresol	106-44-5	901	1025.1	2081.4	2080	C_7H_8O
159	benzene, pentyl-	538-68-1	827	566.1	1407.2	1419	$C_{11}H_{16}$
160	3-hexanone, 5-methyl-	623-56-3	864	241.5	1074.5	1082	$C_7H_{14}O$
161	pyrazine, 2,3-dimethyl-	5910-89-4	925	506.6	1338.6	1344	$C_6H_8N_2$
162	dimethyl trisulfide	3658-80-8	889	536.3	1372.5	1377	$C_2H_6S_3$
163	1-propanone, 1-(2-furanyl)-	3194-15-8	828	695.6	1573.3	1563	$C_7H_8O_2$
164	phenol, 2-methoxy-	90-05-1	931	889.8	1857.8	1861	$C_7H_8O_2$
165	furan, 2-methyl-	534-22-5	946	95.8	881.6	869	C_5H_6O
166	4H-pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	28564-83-2	892	1126.1	2263.8	2267	$C_6H_8O_4$
167	2(5H)-furanone, 3-methyl-	22122-36-7	876	796.1	1714.8	1713	$C_5H_6O_2$
168	thiazole	288-47-1	945	421.3	1246.7	1248	C_3H_3NS
169	2-thiophene carboxaldehyde	98-03-3	948	780.4	1691.8	1684	C_5H_4OS
170	furan, 2-[(methylthio)methyl]-	1438-91-1	857	640.5	1499.7	1491	C_6H_8OS
171	1-propanone, 1-(5-methyl-2-furanyl)-	10599-69-6	801	770.7	1678	1670	$C_8H_{10}O_2$
172	1H-pyrrole-2-carboxaldehyde, 1-methyl-	1192-58-1	905	727.9	1617.5	1626	C_6H_7NO
173	furan, 2,2'-methylenebis-	1197-40-6	909	721.2	1608	1632	$C_9H_8O_2$
174	benzofuran	271-89-6	887	642.0	1501.6	1489	C_8H_6O
175	thiophene, 3-methyl-	616-44-4	916	285.0	1115.1	1122	C_5H_6S
176	pyrazine, 2-ethyl-3-methyl-	15707-23-0	822	556.9	1396	1407	$C_7H_{10}N_2$
177	2-butanone, 4-(5-methyl-2-furanyl)-	13679-56-6	809	793.4	1710.7	1705	$C_9H_{12}O_2$
178	2-furanmethanol	98-00-0	924	757.5	1659.4	1660	$C_5H_6O_2$
179	2-furancarboxaldehyde, 5-methyl-	620-02-0	939	694.6	1572.1	1570	$C_6H_6O_2$
180	1H-pyrrole, 1-(2-furanylmethyl)-	1438-94-4	919	870.2	1827	1824	C_9H_9NO
181	4-cyclopentene-1,3-dione	930-60-9	893	703.9	1584.5	1573	$C_5H_4O_2$
182	maltol	118-71-8	916	955.9	1964.4	1969	$C_6H_6O_3$
183	phenol, 4-ethyl-2-methoxy-	2785-89-9	873	993.1	2026.7	2032	$C_9H_{12}O_2$
184	1-(2-thienyl)-1-propanone	13679-75-9	866	875.5	1835.2	1833	C_7H_8OS
185	2-furanone, 2,5-dihydro-3,5-dimethyl		858	748.2	1646.3	1639	$C_6H_8O_2$
186	ethanone, 1-(3-thienyl)-	1468-83-3	857	834.7	1772.6	1771	C_6H_6OS
187	pyrazine, 2,6-diethyl-	13067-27-1	870	581.6	1426.3	1444	$C_8H_{12}N_2$
188	benzofuran, 2-methyl-	4265-25-2	908	708.5	1590.6	1576	C_9H_8O
189	pyrazine, 2,6-dimethyl-	108-50-9	882	490.7	1320.3	1328	$C_6H_8N_2$
190	pyrazine, ethyl-	13925-00-3	915	496.6	1327.1	1337	$C_6H_8N_2$
191	pyrazine, 2-ethyl-6-methyl-	13925-03-6	906	540.7	1377.5	1386	$C_7H_{10}N_2$
192	3-hexanone	589-38-8	939	216.9	1051.6	1053	$C_6H_{12}O$
193	2-butanone, 1-(2-furanyl)-	4208-63-3	837	713.3	1597	1584	$C_8H_{10}O_2$
194	pyrazine, methyl-	109-08-0	959	434.6	1260.4	1266	$C_5H_6N_2$
195	acetophenone, 4'-hydroxy-	99-93-4	885	851.2	1797.3	1788	$C_8H_8O_2$
196	ethanone, 1-(2-thienyl)-	88-15-3	853	830.3	1766	1763	C_6H_6OS
197	pyrazine	290-37-9	928	383.9	1208	1212	$C_4H_4N_2$
198	2-isobutyl-3-methylpyrazine	13925-06-9	840	625.0	1480.4	1490	$C_9H_{14}N_2$