Application Note

Instrument: Pegasus® BTX and ChromaTOF® Sync

Enhanced Characterization and Comparison of Thyme Varieties from Different Geographical Origins

An Analytical Workflow Solution Combining GC-TOFMS and Automated Statistical Data Processing

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Key Words: Thyme, Herbs, Quality, Non-Target Screening, Natural Products, Supply Chain, Origin, Authenticity, SPME, GC-MS, TOFMS, RI, Deconvolution, Peak Finding, Alignment, ChromaTOF Sync, PCA, Pegasus BTX

Introduction

Understanding the aroma profiles of herbs and spices, or other natural products, is important in the flavor, fragrance, and food industry to assure the quality of raw materials and therefore finished products. The ability to screen multiple materials in depth and efficiently is vital for producers to protect their supply chains and their brands. Comprehending and controlling material properties, quality, and authenticity enhances product development and production optimization, and enables businesses to solve problems faster and react to consumer and market demands.

The volatile and semi-volatile profiles of natural raw materials, such as herbs, can be determined with Gas Chromatography (GC) analysis. Time-of-Flight Mass Spectrometry (TOFMS) is ideal for this type of highly complex analysis due to its full mass range and fast data acquisition capabilities. The Pegasus BTX GC-TOFMS system allows such rich data sets to be collected, providing an enhanced ability to detect and identify scores of significant aroma species.

Comparing analytes and their trends across complex sample sets can be a tedious task. *ChromaTOF* Sync software facilitates this by automatically deconvoluting and statistically processing multiple data sets quickly and efficiently, providing an insightful output of differentiating sample features and characteristics.

In this work, we compared the aroma profiles of dried thyme from different geographical origins (France, Morocco, Poland, and Spain) to understand analyte similarities and differences in the chemical profiles that may impact their aroma.

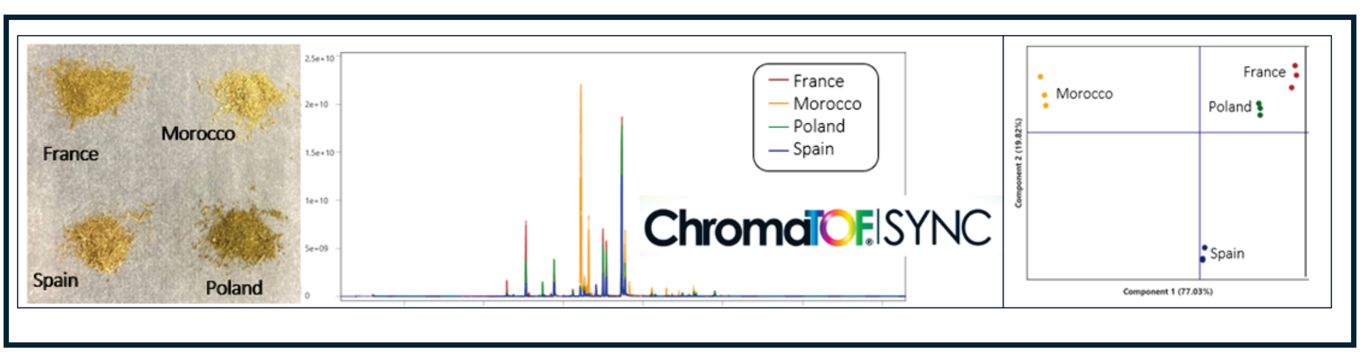


Figure 1. The Pegasus BTX and ChromaTOF Sync are combined to compare dried thyme from four different countries.

Experimental

Thyme samples from different countries (France, Morocco, Poland, and Spain), shown in Figure 1, were analyzed in triplicate with headspace solid phase microextraction (HS-SPME) and GC-TOFMS. For each replicate, 50 mg of dried thyme was measured into a 20 mL headspace vial. The samples were incubated for 2 min at 40 °C in the LPAL-3 agitator and then extracted for 5 min at the same temperature with a tri-phase SPME fiber (PDMS, DVB, CWR). Method details are shown in Table 1. An alkane standard was also analyzed with the same methods to calculate retention index (RI) values.

Table 1. Instrument *(Pegasus* BTX) Conditions

Auto Sampler	**LECO L-PAL 3 Autosampler**
Injection	Desorb for 2 min in GC inlet, split 20:1
Gas Chromatograph	**LECO GC**
Inlet	250 °C
Carrier Gas	He @ 1.4 mL/min
Column	Rxi-5ms, 30 m x 0.25 mm i.d. x 0.25 μm (Restek)
Temperature Program	40 °C (hold 2 min), ramp 10 °C/min to 250 °C (hold 2 min)
Transfer Line	250 °C
Mass Spectrometer	**LECO *Pegasus* BTX**
Ion Source Temperature	250 °C
Mass Range	35-500 m/z
Acquisition Rate	10 spectra/s

Results and Discussion

Comparison and characterization of thyme samples from different origins is significant work because the similarities and differences in their chemical compositions and associated aromas can impact the production and quality of the final product. This in turn affects supply chain costs, consumer perception, and meeting regulatory requirements.

Analysis of the four thyme samples using the *Pegasus* BTX GC-TOFMS system enabled full mass-range, non-target data to be collected at full system sensitivity, revealing highly complex aroma profiles (Figure 2). This rich quality of data allowed deconvolution to be performed successfully, clearly revealing a high number of mass spectrally distinct features, including co-eluting species, which could be identified with high confidence. Furthermore, automated statistical alignment of the data using *ChromaTOF* Sync for data processing facilitated quick and informative trends and patterns across the whole sample set to be easily visualized.

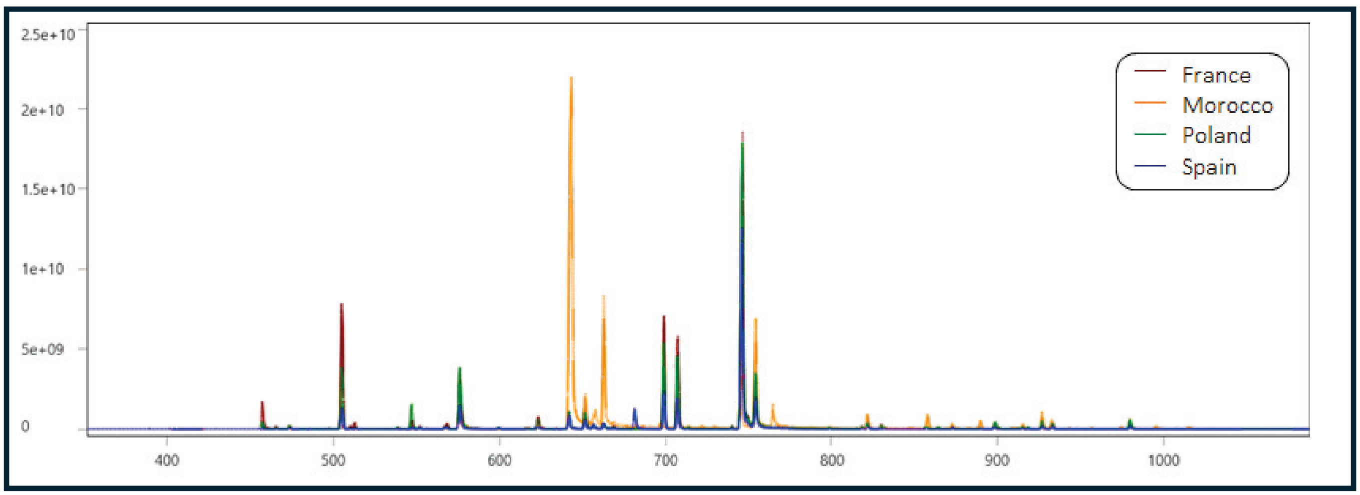


Figure 2. Overlaid full mass range chromatograms for the four thyme varieties.

Identification for these untargeted analytes can often be determined by matching the observed mass spectral (MS) and retention index (RI) data to library databases. For example, the identifications of thymol and carvacrol (Figure 3) were determined with spectral matching to the NIST library database (similarity scores or 851 and 931 for thymol and carvacrol, respectively) and supported by matched RI values (observed RI of 1294 and 1303 compared to library values of 1291 and 1299 for thymol and carvacrol, respectively). The spectral patterns are quite similar for these two analytes, so RI was particularly important in properly assigning the identifications. Confident identifications of these two analytes provided good insights into the samples and the variance in their aromas. Overall trends across the sample set are visually apparent from the overlaid chromatograms (Figure 3), indicating differences in the relative amounts of these analytes in the thyme from different geographical locations. For example, thymol was highest in the thyme from France (maroon) and

Poland (green), medium in the sample from Spain (blue), and lowest in the sample from Morocco (orange). The trends for carvacrol are different, as it was observed at highest levels in the thyme from Morocco relative to the other countries. These trends may be important because the analytes also have interesting aroma notes that likely contribute to the aroma profile of these samples. Thymol is described as herbal with herbal, thyme, phenolic, medicinal, and camphor notes, while carvacrol is described as spicy with spice, woody, camphor, and thymol notes.[1]

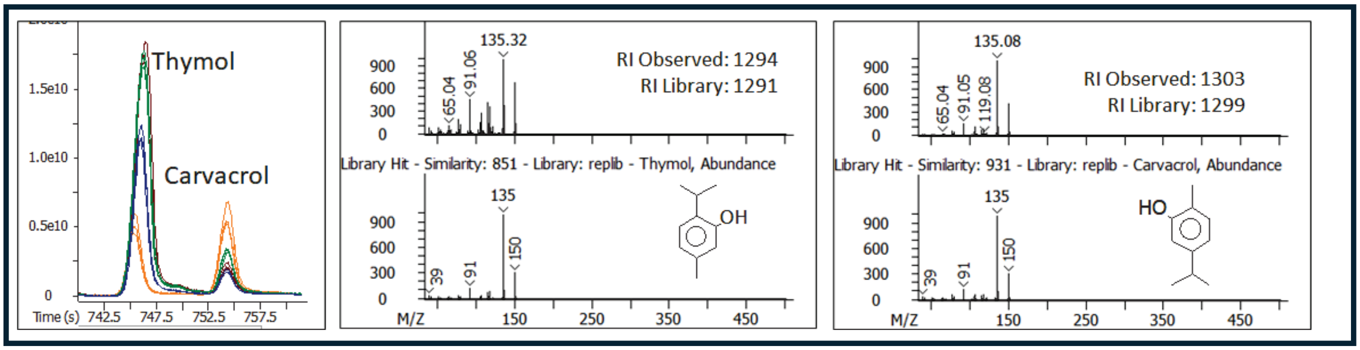


Figure 3. Thymol and carvacrol are identified with library searching of the full m/z data and supported with RI matching to library.

In addition to obtaining full mass range and full sensitivity data, the use of TOFMS also eliminates mass spectral skewing, which can be common and problematic when using scanning instruments. This full mass range non-skewed data further enables efficient use of deconvolution algorithms, which can often mathematically separate coeluting features. For example, 2-pentyl furan and β-myrcene, which chromatographically overlap, were deconvoluted and mathematically separated, extracting clear spectra for each analyte (Figure 4). This allowed confident identifications of both of these analytes, with spectral matching to library databases (similarity scores of 835 and 801 for β-myrcene and 2-pentyl furan, respectively) and RI support (observed RI of 992 and 993 compared to library values of 991 and 993 for β-myrcene and 2-pentyl furan, respectively).

The individual chromatographic profiles and trends across the sample set were easily observed by plotting XICs for each, m/z 93.07 for β-myrcene and m/z 138.11 for 2-pentyl furan. β-myrcene is observed at higher levels in the thyme from Poland and France compared with the samples from Spain and Morocco. 2-pentyl furan was observed at comparable levels in the thyme from Poland, France, and Spain, but at lower levels in the thyme from Morocco. These trends may be important as these analytes have contrasting aroma notes that likely contribute to the overall aroma profiles of the thyme samples. β-myrcene has spicy aroma notes with peppery, terpene, spicy, balsam, and plastic descriptors. 2-pentyl furan is fruity with fruity, green, earthy, beany, vegetable, and metallic notes.[1]

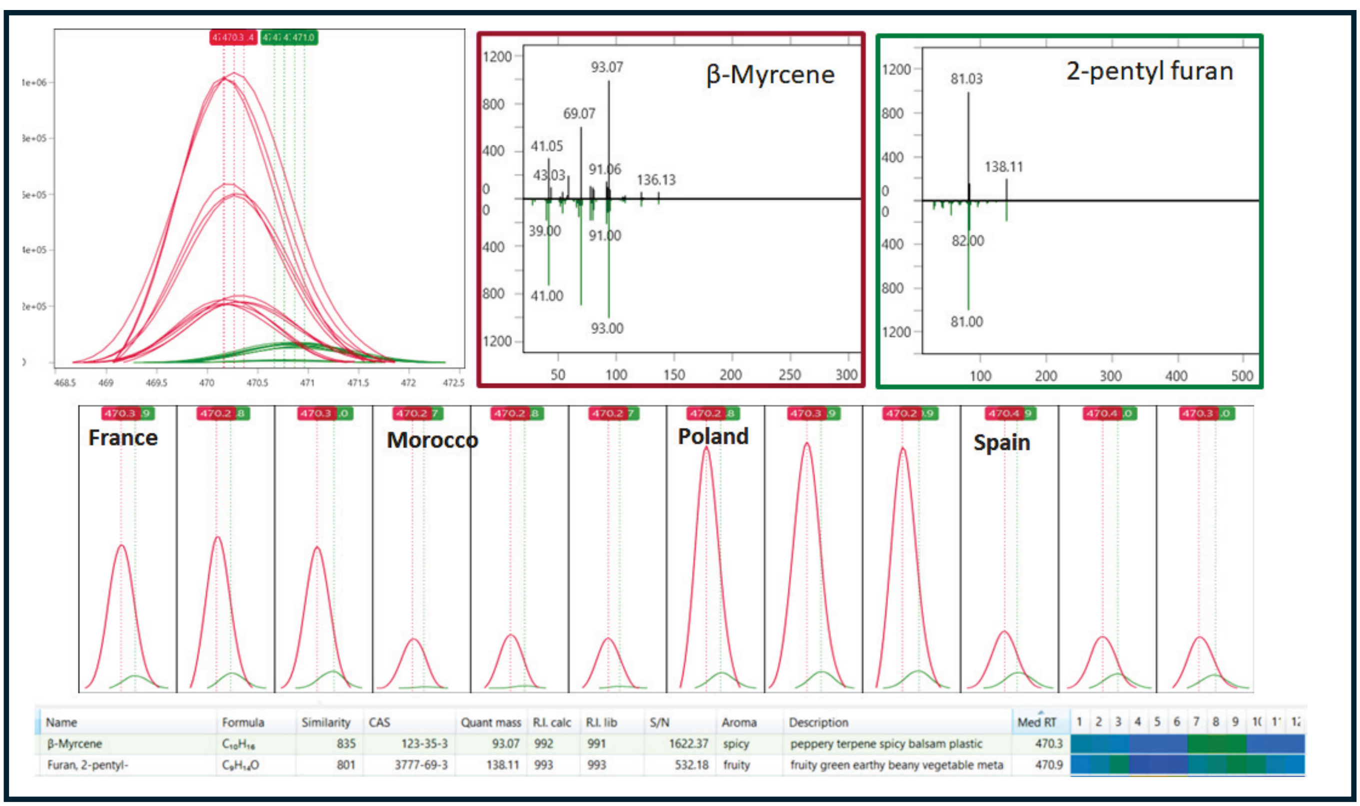


Figure 4. Beta-myrcene and 2-pentyl furan chromatographically overlap and are mathematically separated with deconvolution.

Non-target analyte detectability was excellent and a high number of trace level species were found due to the highly sensitive mass spectral detection of the BTX TOFMS system. Many low-level features are buried in the background and not easily visible in the TIC, so automated peak finding and deconvolution were valuable for isolating the spectral information in these instances. For example, an analyte identified as 2-hexanone (Figure 5), was not visible in the TIC, but deconvolution isolated spectral information that matched to library with a similarity score of 859. The 2-hexanone identification was further supported with an observed RI value of 795 compared to the library value of 790. Even though the feature was hidden in the TIC, the peak profile and quantitative trends were observed by automatic ion extraction of the unique XIC, m/z 100.09. This analyte was observed at higher levels in the thyme from France and Poland and at lower levels in the thyme from Morocco and Spain. These differences may be important as the analyte has fruity aroma characteristics.[1] Additionally, the odor strength is listed as high,[1] suggesting that even low levels of this compound may impact the overall aroma characteristics and contribute to the differences between the samples.

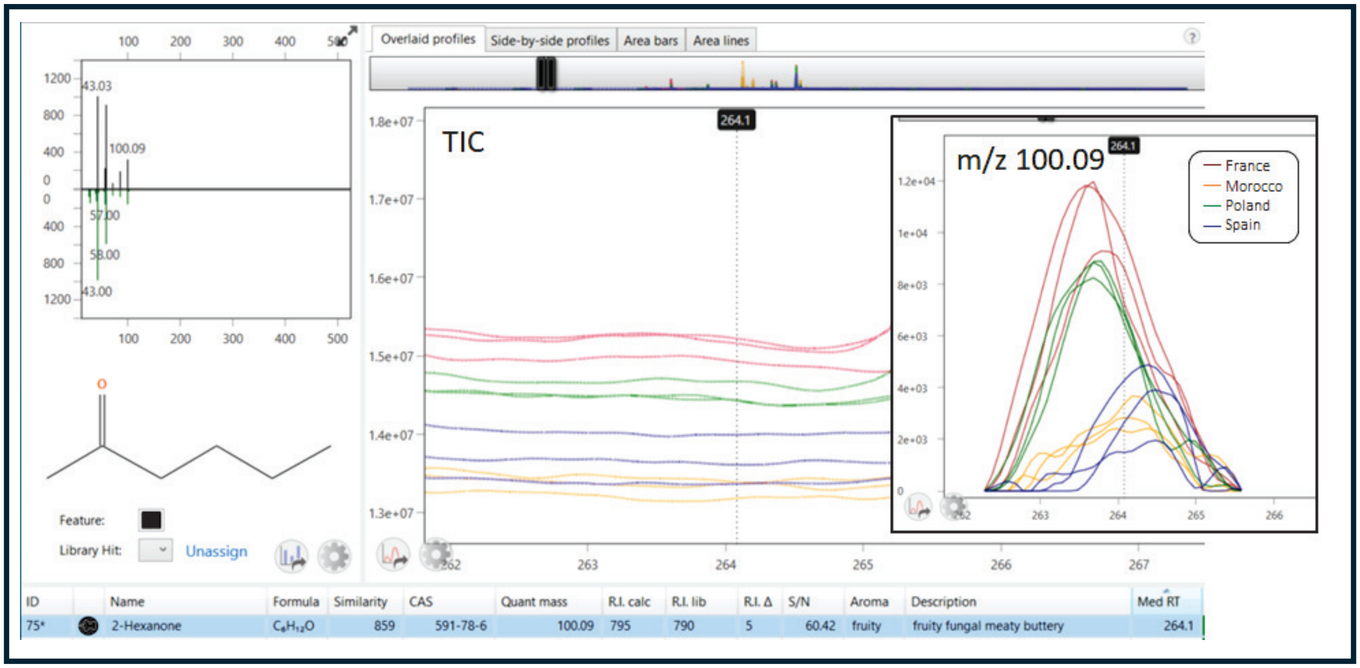


Figure 5. Sensitive detection and automated peak finding reveal low-level analytes that may not be visible in the TIC.

Aligning and statistically comparing the multitude of features within the rich, non-target data from the *Pegasus* BTX TOFMS system could be quite a tedious task in a multi-sample and replicate analysis. Here, the use of *ChromaTOF* Sync significantly increased the speed and output quality of this process.

For example, multi-replicate and sample results for thymol and carvacrol are informatively displayed together with *ChromaTOF* Sync (Figure 6). The peak table includes peak areas for all 12 samples making it easier to determine trends across the sample set. The peak area trends are visualized as overlaid chromatographic profiles, together with side-by-side chromatographic profiles, bar charts (line charts are also an option), and via color deviations in the heat map of the peak table.

Figure 6. Peak information is compiled for the entire sample set with ChromaTOF Sync. Thymol (left) and carvacrol (right) are shown.

Principal Component Analysis (PCA) was also performed with the compiled peak information and overall trends between the samples were determined. The scores plot (Figure 7, left) represents each sample replicate as a data point. The samples that are closest to each other are more similar and those further from each other are more distinct. It enables an easy results overview to be visualized; thyme from Morocco and thyme from Spain are quite distinct, while thyme from Poland and France are more similar to each other. The associated loadings plot (Figure 7, right) reveals how the analytes (variables) contribute to these overall trends, which can then be investigated in more detail. For example, the levels of differentiation of four representative analytes (labeled A, B, C, D on the loadings plot) are displayed (Figure 8). This workflow enables analyte features contributing to significant sample deviations to be seen easily, and possible identifications using mass spectral and RI matching to libraries to be reviewed.

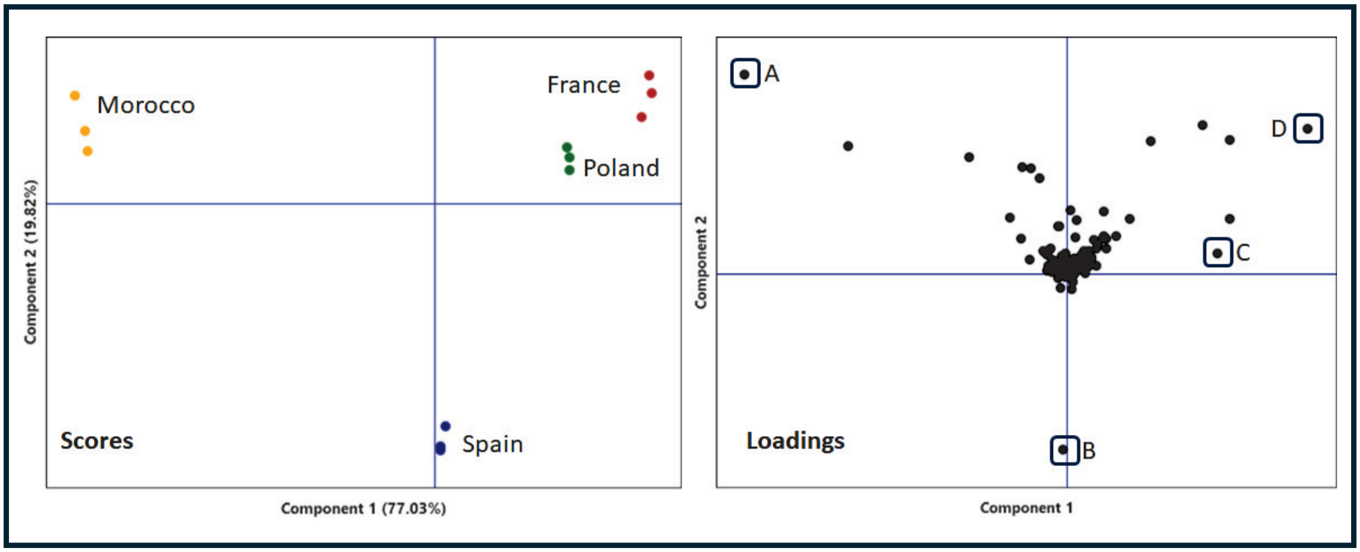


Figure 7. PCA scores and loadings.

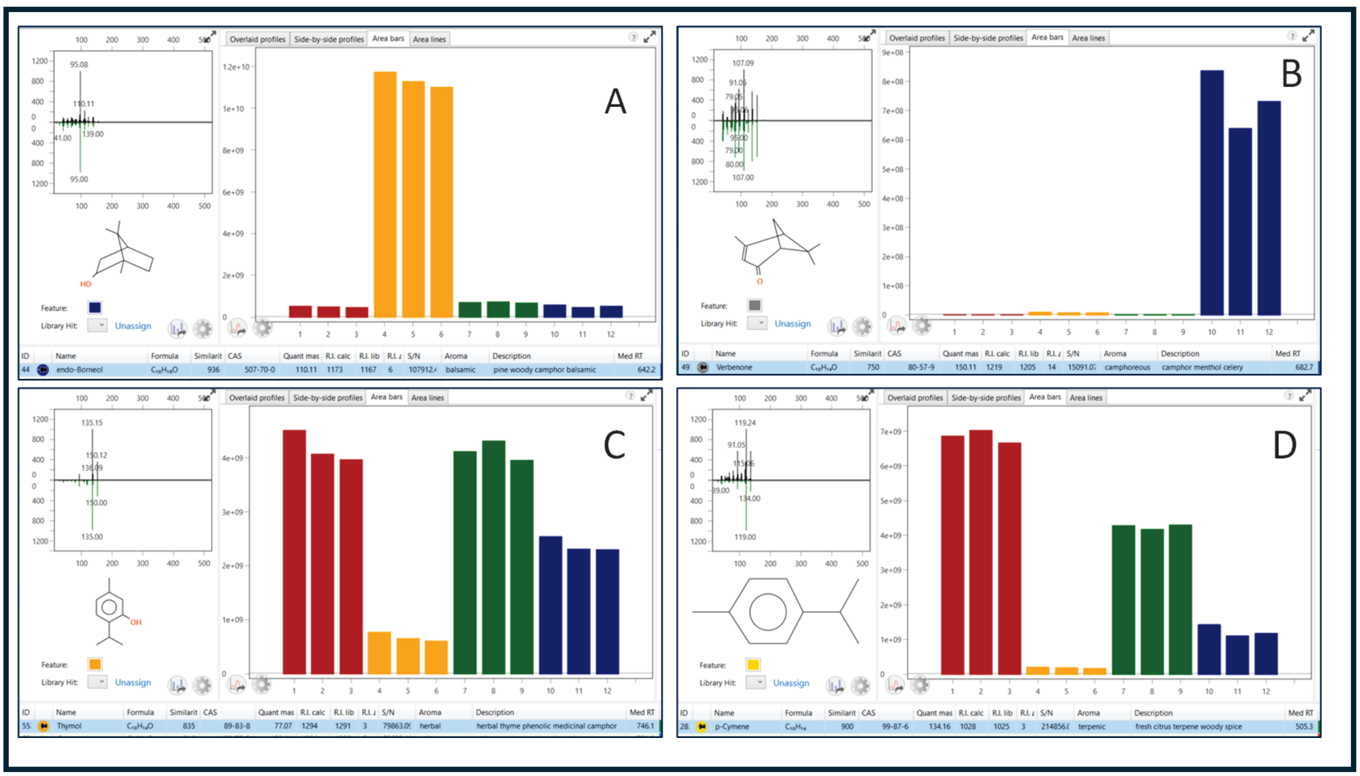


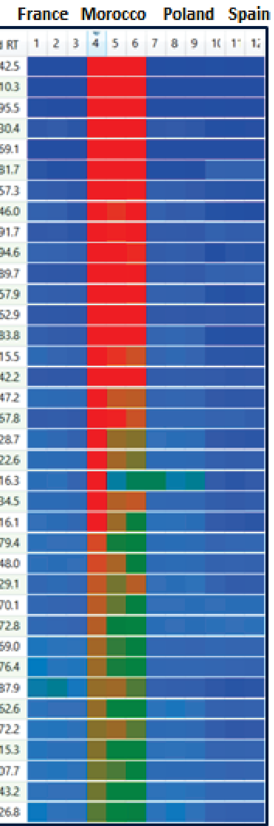
Figure 8. Representative analytes with distinct trends.

The heatmap feature in the peak table also allowed the large number of analytes found in the thyme samples to be viewed together, enabling highly efficient data interpretation and focus. The peak tables can be sorted by heatmap for each country, so analytes that were observed as elevated in the thyme from Morocco (Table 2), for example, are shown as "hotter" (red) in the top section of the table. Other representative analytes, sorted by heat map for France, Poland and Spain, are also provided (Appendix A).

This feature allows fast navigation through the peak table and focus to be drawn to relevant details, which differentiate the thyme sample. For example, the thyme from Morocco tended to have higher levels of terpenes and terpenoids and many of the analytes had woody aroma descriptors. The thyme from Spain had fewer analytes that were very distinct, but those that were tended to have consistent aroma descriptors with camphor or minty notes. Many of the analytes that were elevated in the thyme from Poland were also elevated in the thyme from France. This was consistent with the close proximity of Poland and France on the PCA scores plot. There were more nitrogen-containing compounds in this group, some with nutty aroma descriptors. The thyme from France had more functional group variability in the analytes observed at higher levels, including more esters, carboxylic acids, and alcohols.

Table 2. Representative analytes displayed in a section of the peak table, sorted by heat map for Morocco

Name	Formula	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	S/N	Aroma	Description	Med RT
Kaur-16-ene, (8β,13β)-	$C_{20}H_{32}$	827	20070-61-5	272.26	2027	2012	811.35			1242.5
δ-Guaiene	$C_{15}H_{24}$	819	3691-11-0	204.19	1506	1505	222.71			910.3
α-Terpinyl acetate	$C_{12}H_{20}O_2$	810	80-26-2	136.13	1356	1350	536.39	herbal	herbal bergamot lavender lime citrus	795.5
1,7-Octadiene-3,6-diol, 2,6-di	$C_{10}H_{18}O_2$	866	51276-33-6	137.10	1276	1274	1191.53			730.4
Cyclohexene, 6-ethenyl-6-met	$C_{15}H_{24}$	808	5951-67-7	161.14	1451	1454	913.24			869.1
Aromadendrene, dehydro-	$C_{15}H_{22}$	772		159.12	1468	1464	1881.26			881.7
Ethanone, 1-(4-methylphenyl)	$C_9H_{10}O$	752	122-00-9	67.06	1190	1183	4064.62	floral	hawthorn sweet mimosa coumarin cherry acetophenone	657.3
2,4-Hexadiene, (E,E)-	C_6H_{10}	896	5194-51-4	82.08	637	646	450.25			146.0
Bicyclo(3.1.1)heptane-2,3-diol	$C_{10}H_{18}O_2$	764	53404-49-2	126.11	1230	1244	4430.03			691.7
2(5H)-Furanone	$C_4H_4O_2$	885	497-23-4	84.02	920	920	968.76	buttery	buttery	394.6
(1R,9R,E)-4,11,11-Trimethyl-8-	$C_{15}H_{24}$	834	68832-35-9	204.19	1478	1466	8326.02			889.7
Caryophyllene	$C_{15}H_{24}$	781	87-44-5	133.11	1436	1419	13127.44	spicy	sweet woody spice clove dry	857.9
α-Terpineol	$C_{10}H_{18}O$	913	98-55-5	136.13	1196	1189	52909.60	terpenic	pine terpene lilac citrus woody floral	662.9
Humulene	$C_{15}H_{24}$	791	6753-98-6	93.07	1470	1454	2072.73	woody	woody	883.8
10,10-Dimethyl-2,6-dimethyle	$C_{15}H_{24}O$	791	19431-80-2	136.10	1657	1644	1520.80			1015.5
endo-Borneol	$C_{10}H_{18}O$	936	507-70-0	110.11	1173	1167	107912.44	balsamic	pine woody camphor balsamic	642.2
cis-Caryophyllene	$C_{15}H_{24}$	914	118-65-0	161.14	1422	1406	1332.74	woody	woody spicy	847.2
Palustrol	$C_{15}H_{26}O$	855	5986-49-2	204.19	1587	1568	469.94			967.8
14-Hydroxycaryophyllene	$C_{15}H_{24}O$	865	50277-33-3	187.16	1677	1686	562.98			1028.7
Carvenone	$C_{10}H_{16}O$	894	499-74-1	152.12	1266	1257	4231.08	mint	spearmint	722.6
Methacrolein	C_4H_6O	873	78-85-3	70.04	565	567	1216.07	floral	wild hyacinth foliage	116.3
Isoborneol	$C_{10}H_{18}O$	881	124-76-5	95.09	1165	1157	5667.89	balsamic	balsam camphor herbal woody	634.5
.tau.-Cadinol	$C_{15}H_{26}O$	881	5937-11-1	161.14	1658	1640	4049.05	balsamic	balsamic earthy	1016.1
4,11,11-trimethyl-8-methylene	$C_{15}H_{24}$	864	889360-49-	189.18	1464	1460	422.93			879.4
α-Calacorene	$C_{15}H_{20}$	805	21391-99-1	157.11	1559	1542	5852.46	woody	woody	948.0
Camphene	$C_{10}H_{16}$	841	79-92-5	121.10	953	952	3332.04	woody	woody herbal fir needle camphor terpenic	429.1
α-Maaliene	$C_{15}H_{24}$	859	489-28-1	122.11	1452	1443	1340.18			870.1
Alloaromadendrene	$C_{15}H_{24}$	919	25246-27-9	204.19	1456	1461	6721.90	woody	woody	872.8
trans-Dihydrocarvone	$C_{10}H_{16}O$	919	5948-04-9	152.12	1203	1201	1851.73	herbal	warm herbal	669.0
(+)-Dihydrocarvone	$C_{10}H_{16}O$	769	5524-05-0	152.12	1212	1210	575.25	minty	herbal minty mentholic	676.4
(2R,5S)-2-Methyl-5-(prop-1-e	$C_{10}H_{16}O$	750	54750-69-5	137.10	1010	1008	804.27			487.9
β-Calacorene	$C_{15}H_{20}$	899	50277-34-4	157.11	1580	1563	1810.88			962.6
2,3-Dehydro-1,8-cineole	$C_{10}H_{14}O$	753	92760-25-3	109.08	994	991	1511.85	minty	mint lemon	472.2
α-Muurolene	$C_{15}H_{24}$	867	10208-80-7	204.19	1513	1499	7253.13	woody	woody	915.3
3-Furaldehyde	$C_5H_4O_2$	924	498-60-2	95.01	837	831	3928.77			307.7
α-Cadinene	$C_{15}H_{24}$	915	24406-05-1	204.19	1552	1538	2490.50	woody	woody dry	943.2
δ-Cadinene	$C_{15}H_{24}$	837	483-76-1	161.14	1529	1524	24714.91	herbal	thyme herbal woody dry	926.8



Conclusion

In this work, the *Pegasus* BTX GC-TOFMS system and *ChromaTOF* Sync were used to evaluate and compare dried thyme samples from four different countries; France, Morocco, Poland, and Spain. Rich, non-target data with full mass range acquisition and enhanced sensitivity was collected, allowing efficient deconvolution and excellent analyte detection coverage across these complex samples. *ChromaTOF* Sync efficiently aligned and compiled analyte information across the sample set, facilitating the comparison and interpretation. Many distinct analytes with interesting aroma notes were observed in each of the thyme samples, and alignment allowed links between these differentiating chemicals to be made with the origins of the four thyme varieties.

Much of the sample preparation was automated with an LPAL-3 auto sampler and *ChromaTOF* Software, which also controls the GC and MS operation. Additionally, the Pegasus BTX has a StayClean™ Ion Source, which eliminates the downtime associated with source cleaning—a quality of high importance for the robust, routine analysis of multiple samples.

This efficient, full workflow solution demonstrates an ability to quickly gain important insights, which can help producers in the consumer goods sector to develop better products, understand the competition, and respond quickly to resolve quality, supply, or manufacturing issues.

Acknowledgement

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References

[1]Good Scents database, http://www.thegoodscentscompany.com

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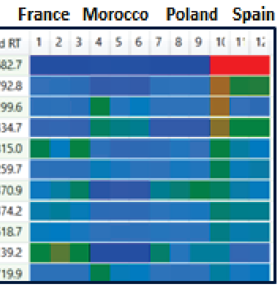
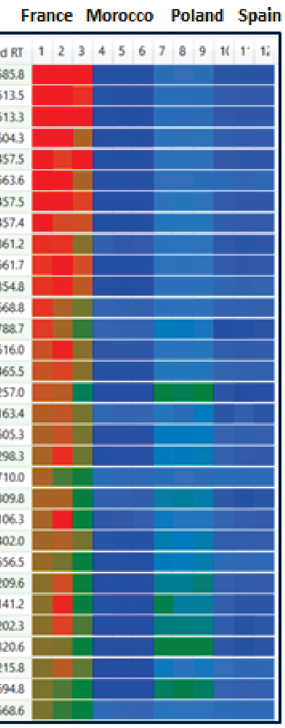
Appendix A

Peak table sections, with representative analytes, sorted by heat map for thyme samples from Spain, Poland and France.

Name	Formula	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	S/N	Aroma	Description	Med RT
Verbenone	$C_{10}H_{14}O$	750	80-57-9	150.11	1219	1205	15091.07	camphoreous	camphor menthol celery	682.7
2-Cyclohexen-1-one, 3-methy	$C_{10}H_{14}O$	767	491-09-8	150.11	1352	1340	636.36	minty	sharp minty phenolic	792.8
Acetone	C_3H_6O	867	67-64-1	58.04	499	487	1302.41	solvent	solvent ethereal apple pear	99.6
Bicyclo[3.1.0]hex-2-ene, 4-me	$C_{10}H_{14}$	858	36262-09-6	91.05	958	956	2112.05			434.7
Propanoic acid, 2-methyl-, 3-l	$C_{12}H_{24}O_3$	836	77-68-9	173.13	1380	1374	489.38			815.0
2-Butenal, 3-methyl-	C_5H_8O	763	107-86-8	84.06	790	782	410.21	fruity	sweet fruity pungent brown nutty almond cherry	259.7
Furan, 2-pentyl-	$C_9H_{14}O$	801	3777-69-3	138.11	993	993	532.18	fruity	fruity green earthy beany vegetable metallic	470.9
Benzene, 1,2,4-trimethyl-	C_9H_{12}	768	95-63-6	120.10	996	990	442.68	plastic	plastic	474.2
2,6,6-Trimethyl-2-cyclohexene	$C_9H_{12}O_2$	777	1125-21-9	152.09	1148	1145	796.29	musty	musty woody sweet tea tobacco leaf	618.7
1-Propanol, 2-methyl-	$C_4H_{10}O$	831	78-83-1	74.07	625	624	21.80	ethereal	etherael winey corex	139.2
2-Cyclohexen-1-one, 3-methy	$C_{10}H_{16}O$	806	89-81-6	82.04	1263	1253	809.39	herbal	herbal minty camphor medicinal	719.9



Name	Formula	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	S/N	Aroma	Description	Med RT
1-Octen-3-yl-acetate	$C_{10}H_{18}O_2$	840	2442-10-6	99.05	1111	1111	3261.29	herbal	fresh green herbal lavender fruity oily	585.8
Benzyl alcohol	C_7H_8O	754	100-51-6	108.06	1036	1036	8007.68	floral	floral rose phenolic balsamic	513.5
Eucalyptol	$C_{10}H_{18}O$	914	470-82-6	154.14	1036	1032	13243.27	herbal	eucalyptus herbal camphor medicinal	513.3
(2R,4R)-4-Methyl-2-(2-methyl	$C_{10}H_{18}O$	817	5258-11-7	139.12	1132	1127	819.50	floral	flower	604.3
Phenol	C_6H_6O	826	108-95-2	66.05	980	981	3707.14	phenolic	phenolic plastic rubber	457.5
3-Nonanone	$C_9H_{18}O$	808	925-78-0	113.10	1088	1090	663.07	floral	fresh sweet jasmin spicy leaf herbal fruity	563.6
1-Octen-3-ol	$C_8H_{16}O$	886	3391-86-4	57.04	980	980	37135.41	earthy	mushroom earthy green oily fungal raw chicken	457.5
1-Octen-3-one	$C_8H_{14}O$	773	4312-99-6	70.04	980	979	8714.83	earthy	herbal mushroom earthy musty dirty	457.4
3-Methyl-3-buten-1-ol, acetat	$C_7H_{12}O_2$	906	5205-07-2	68.06	888	881	1303.55	fruity	fruity	361.2
Benzene, 1-methyl-3-(1-meth	$C_{10}H_{12}$	937	1124-20-5	132.10	1086	1082	4246.23			561.7
1-Hepten-3-ol	$C_7H_{14}O$	799	4938-52-7	57.04	882	883	338.42	green	oily green metallic acrylate tomato spicy	354.8
Estragole	$C_{10}H_{12}O$	920	140-67-0	148.09	1203	1196	8781.20	anisic	sweet sassafrass anise spice green herbal fennel	668.8
δ-Elemene	$C_{15}H_{24}$	867	20307-84-0	161.14	1347	1338	1168.45	herbal	sweet herbal woody	788.7
Cyclohexanone, 2,2,6-trimethy	$C_9H_{16}O$	812	2408-37-9	140.12	1039	1036	1126.71	thujonic	pungent thujone labdanum honey cistus	516.0
3-Octanone	$C_8H_{16}O$	842	106-68-3	99.08	988	986	4063.06	herbal	fresh herbal lavender sweet mushroom	465.5
2,3-Butanediol	$C_4H_{10}O_2$	851	513-85-9	45.05	787	788	149.47	creamy	fruity creamy buttery	257.0
2-Propanone, 1-hydroxy-	$C_3H_6O_2$	866	116-09-6	74.04	668	666	106.87	caramellic	pungent sweet caramellic ethereal	163.4
1-Hexanol, 2-ethyl-	$C_8H_{18}O$	827	104-76-7	57.07	1028	1030	4294.69	citrus	citrus fresh floral oily sweet	505.3
Methyl valerate	$C_6H_{12}O_2$	807	624-24-8	74.03	828	823	414.99	fruity	sweet green fruity apple pineapple nutty	298.3
D-Carvone	$C_{10}H_{14}O$	896	2244-16-8	82.04	1251	1246	10373.97	minty	spice mint bread caraway	710.0
Butanoic acid, 3-methyl-	$C_5H_{10}O_2$	868	503-74-2	87.04	839	850	1387.62	cheesy	sour stinky feet sweaty cheese tropical	309.8
Acetic acid, methyl ester	$C_3H_6O_2$	939	79-20-9	74.03	525	526	374.72	ethereal	ether sweet fruity	106.3
Hexanoic acid, methyl ester	$C_7H_{14}O_2$	822	106-70-7	99.08	927	925	1029.27	fruity	ethereal fruity pineapple apricot strawberry tropical fruity	402.0
1-Nonen-3-ol	$C_9H_{18}O$	873	21964-44-3	57.04	1080	1080	4326.96	earthy	intensely oily creamy green earthy mushroom	556.5
3-Buten-1-ol, 3-methyl-	$C_5H_{10}O$	923	763-32-6	86.07	732	731	1477.27	fruity	sweet fruity	209.6
Methyl propionate	$C_4H_8O_2$	923	554-12-1	88.05	628	627	257.21	fruity	fresh harsh rum fruity strawberry apple	141.2
Butanoic acid, methyl ester	$C_5H_{10}O_2$	836	623-42-7	71.05	724	723	349.55	fruity	fruity apple sweet banana pineapple	202.3
Butanoic acid, 2-methyl-	$C_5H_{10}O_2$	909	116-53-0	74.04	849	861	6867.58	acidic	pungent acid roquefort cheese	320.6
1-Butanol, 2-methyl-	$C_5H_{12}O$	880	137-32-6	57.07	740	739	498.12	ethereal	ethereal fusel alcoholic fatty greasy winey whiskey leather	215.8
Benzene, 1-methoxy-4-methy	$C_{11}H_{16}O$	809	31574-44-4	149.10	1234	1230	601.09			694.8
Benzene, 1-methyl-4-(1-meth	$C_{10}H_{12}$	917	1195-32-0	132.10	1093	1090	22780.20	phenolic	phenolic spicy styrene clove guaiacol	568.6



Name	Formula	Similarity	CAS	Quant mass	R.I. calc	R.I. lib	S/N	Aroma	Description	Med RT
1,2-Ethanediol	$C_2H_6O_2$	843	107-21-1	62.04	698	702	3720.04			180.7
Pyrazine	$C_4H_4N_2$	902	290-37-9	80.04	742	736	1945.59	nutty	pungent sweet corn like roasted hazelnut barly	218.1
(1R,5R)-2-Methyl-5-((R)-6-me	$C_{15}H_{24}$	848	58319-06-5	119.09	1411	1402	278.60			839.5
cis-4-Thujanol	$C_{10}H_{18}O$	846	15537-55-0	136.13	1071	1070	21474.99	balsamic	balsam	547.5
1-Heptanol	$C_7H_{16}O$	774	111-70-6	70.08	972	970	1051.44	green	musty leafy violet herbal green sweet woody peony	448.5
Pyrazine, methyl-	$C_5H_6N_2$	941	109-08-0	94.05	832	829	2263.81	nutty	nutty cocoa roasted chocolate peanut green	302.1
Butanoic acid, 2-methyl-, met	$C_6H_{12}O_2$	833	868-57-5	101.06	781	775	461.78	fruity	ethereal estery fruity tutti frutti green apple lily of the valle	251.7
β-Bisabolene	$C_{15}H_{24}$	897	495-61-4	109.10	1517	1509	3159.55	balsamic	balsamic woody	918.2
3-Heptanol	$C_7H_{16}O$	808	589-82-2	59.05	898	877	335.59	herbal	powerful herbal	371.9
Sabinene	$C_{10}H_{16}$	958	3387-41-5	136.13	977	974	3226.69	woody	woody terpene citrus pine spice	454.3
Bicyclo[3.1.0]hex-2-ene, 2-me	$C_{10}H_{16}$	934	2867-05-2	93.07	930	929	5319.51	woody	woody green herb	405.7
1-Hexanol	$C_6H_{14}O$	878	111-27-3	56.07	871	868	3509.48	herbal	ethereal fusel oil fruity alcoholic sweet green	344.0
Pyrazine, 2-ethyl-6-methyl-	$C_7H_{10}N_2$	754	13925-03-6	121.08	1005	1003	153.92	potato	roasted potato	483.0
γ-Terpinene	$C_{10}H_{16}$	838	99-85-4	136.13	1063	1060	8257.97	terpenic	oily woody terpene lemon/lime tropical herbal	539.1
Pyrazine, 2,3-dimethyl-	$C_6H_8N_2$	892	5910-89-4	108.07	926	920	456.11	nutty	nutty nut skin cocoa peanut butter coffee walnut caramelli	400.9
1,3-Cyclohexadiene, 1-methyl	$C_{10}H_{16}$	765	99-86-5	121.12	1020	1017	5102.42	woody	woody terpene lemon herbal medicinal citrus	497.7
4-Hexen-1-ol, 5-methyl-2-(1-	$C_{10}H_{18}O$	767	498-16-8	124.12	1170	1170	382.95	herbal	herbal	638.8
γ-Eudesmol	$C_{15}H_{26}O$	767	1209-71-8	189.17	1642	1631	441.25	waxy	waxy sweet	1005.3
Benzene, 1,3,5-trimethoxy-	$C_9H_{12}O_3$	885	621-23-8	168.09	1415	1392	2443.53			842.5
β-Myrcene	$C_{10}H_{16}$	835	123-35-3	93.07	992	991	1622.37	spicy	peppery terpene spicy balsam plastic	470.3
β-Yalangene	$C_{15}H_{24}$	909	20479-06-5	161.14	1434	1421	3070.27			856.3
Pyridine, 2-ethyl-	C_7H_9N	954	100-71-0	106.07	916	906	1503.85	green	green grassy	390.7
2,4-Heptadienal, (E,E)-	$C_7H_{10}O$	828	4313-03-5	81.04	996	1012	343.71	fatty	fatty green oily aldehydic vegetable cake cinnamon	473.9
3-Heptanone	$C_7H_{14}O$	836	106-35-4	114.11	889	887	139.72	green	powerful green fatty fruity	362.6
2,3-Butanediol	$C_4H_{10}O_2$	851	513-85-9	45.05	787	788	149.47	creamy	fruity creamy buttery	257.0
Pentanal	$C_5H_{10}O$	902	110-62-3	58.04	699	700	771.48	fermented	fermented bready fruity nutty berry	180.9
3-Octanol	$C_8H_{18}O$	923	589-98-0	101.10	996	993	8100.32	earthy	earthy mushroom herbal melon citrus woody spicy minty	473.9
3-Hexen-2-one	$C_6H_{10}O$	839	763-93-9	83.05	846	845	777.51			317.2
α-Amorphene	$C_{15}H_{24}$	878	20085-19-2	204.20	1493	1483	1000.83			901.2
1-Pentanol	$C_5H_{12}O$	925	71-41-0	70.08	770	765	1270.64	fermented	fusel oil sweet balsam	242.3
Benzene, 2-methoxy-4-methy	$C_{11}H_{16}O$	927	1076-56-8	91.05	1239	1235	40370.64	herbal	woody smoky burnt	699.1
Cyclohexene, 1-methyl-4-(1-n	$C_{10}H_{16}$	858	586-62-9	134.11	1101	1088	5780.02	herbal	fresh woody sweet pine citrus	576.6