Application Note

Flavors and Fragrances

Agilent

Trusted Answers

Profiling Flavors and Fragrances in Complex Matrices Using Linear Retention Indices Without Sample Preparation

Author

Eleazar Rojas Santiago
Agilent Technologies, Inc.

Abstract

This Application Note describes a method for the analysis of flavor and fragrance compounds. The method deploys gas chromatography/mass spectrometry (GC/MS) using backflush and a thermal separation probe at constant flow with an Agilent Intuvo 9000 GC and an Agilent 5977B GC/MSD. Flavor and fragrance compounds in complex matrices such as soap, scented candles, toothpaste, body lotion, and fabric softener were analyzed without sample preparation. The samples were introduced into the GC/MSD system using the thermal separation probe. Identification was done using deconvoluted mass spectra and incorporating linear retention index results. In addition, a hyperlink was created to connect the compound name with a fragrance and flavor website to obtain organoleptic and cosmetic information.

Introduction

The Agilent Thermal Separation Probe (TSP) is ideal for fast GC/MS analysis of a variety of dirty liquid and solid samples in food testing, forensics, and environmental applications. Advantages of the thermal separation probe include:

- Little or no sample preparation required
- Greater flexibility with less risk than traditional direct sample probes
- Low risk of contamination or decrease in performance typically associated with traditional direct sample probes
- Control sample delivery by adjusting split flow ratios, eliminating the possibility of overload or contamination of the detector
- Temperature programming in the inlet and GC column for improved identification of multicomponent samples, which is not possible with traditional direct sample probes
- Two ways to use TSP with GC/MS systems: separate complex samples using a longer analytical column, or transfer the neat sample to the MS using a short deactivated capillary column

GC/MS has been used for many years for the analysis of fragrance and flavor compounds[1]. GC/MS is probably the most powerful technique, and extended mass spectral libraries are available, but do not enable complete identification. In flavor and fragrance quality control, GC/MS with retention indices (RIs) is still frequently used as a complementary technique to GC/MS. Several libraries are available with RIs for many flavor and fragrance compounds[2-4]. RIs are less dependent on operational parameters than absolute retention times, but they still depend significantly on the column type (stationary phase and supplier), temperature program, and, to a lesser extent, on the carrier gas velocity. Therefore, it is sometimes difficult to reproduce published RIs in different laboratories. Most companies in the flavor and fragrance industry use in-house methods based on historical choices of columns and conditions.

Agilent MassHunter Unknowns Analysis software uses a deconvolution process that helps identify compounds even when they are hidden under coeluting matrix compounds. The deconvolution process is automated, and takes approximately 1 to 2 minutes for a total ion chromatogram (TIC). The process not only allows analysts to get reliable and reproducible results fast, but also minimizes false positives and false negatives[5].

Because many retention data are already available as RIs, it was also evaluated whether these data could be transferred into absolute retention times that match with locked retention times. It was shown that RIs from existing retention index libraries can be recalculated as absolute retention times that match with experimental data. In this study, two libraries with RIs were used: NIST 2017, and the Agilent flavor and fragrance RTL library[6].

The innovations in the Intuvo 9000 GC include:

- A direct heating system, which is faster, uses half the power, and takes half the bench space of a conventional air-bath oven
- Ferrule-free direct connections with a plug-and-play flowpath eliminate a major source of complexity and leaks.
- The unique disposable Intuvo Guard Chip eliminates the need for column trimming.

Experimental

Analyses were performed on an Intuvo 9000 GC equipped with a multimode inlet (MMI) and post column backflush. The MMI was set to 60 °C to introduce the TSP at a low temperature, thus avoiding loss of light components before the actual injection occured. After introducing the TSP, the MMI temperature was ramped to 280 °C at 600 °C/min. Separation was done on an Agilent HP-5MS, 30 m × 0.25 mm id, 0.25 µm column (β = 250) (p/n 19091S-433-INT). Helium at approximately 65 kPa (9.43 psi) at constant flow was used as the carrier gas. Table 1 summarizes the analytical conditions.

Table 1. GC/MS analytical conditions.

Parameter	Description
Column	HP-5MS, 30 m × 0.25 mm id, 0.25 µm (p/n 19091S-433-INT)
Injection	MMI, split ratio 100:1, 0.2 minutes 40 °C, then 900 °C/min to 300 °C
Carrier gas	Helium (13.4 psi), constant flow
RTL	Flow set to 1.46 mL/min to give a retention time of 32.000 minutes for *n*-hexadecane
Oven program	60 to 240 °C at 3 °C/min (60 minutes analysis time)
Guard Chip	Intuvo, multimode inlet
Temperature program	Track oven
Detection	MSD XTR 6 mm in scan mode (40 to 400 amu) solvent delay: 0 minutes transfer line: 300 °C

An alkanes mix from C_6 to C_{44} was injected using the conditions described in Table 2 to generate the calibration retention time (CRT) file, and MassHunter was used to analyze the file and calculate library retention times.

Data were processed with MassHunter Unknowns Analysis software, using a deconvolution process and RIs from two libraries. The software calculates the library retention time using the CRT file and the RI from the different libraries, and calculates the difference between library retention time and real retention time. By applying the retention time filter and the minimum match factor, it was possible to eliminate misidentification.

Table 2. MassHunter Unknowns Analysis method parameters.

Parameter	Description
RT window size factor	25, 50, 100, 200
Peak filter SNR threshold	5
Match factor (RT penalty)	Enable Trapezoidal RT range: 60 seconds Penalty free RT range: 30 seconds
Min match factor	75
Library search type	Spectral search

Transformation of RIs

The linear retention index (LRI) requires that an n-alkane mixture is analyzed in the elution range of the analytes of interest. Each n-alkane is assigned an LRI value based on the number of carbon atoms multiplied by 100. For example, octane (n-C_8) is assigned an LRI of 800, nonane (n-C_9) is assigned an LRI of 900, decane (n-C_{10}) is assigned an LRI value of 1,000, and so on. The LRI of a given analyte was calculated according to where it elutes relative to the n-alkanes that eluted immediately before and after the analyte.

For temperature-programmed GC, the LRI is calculated by the following equation:

$$I = 100 \times \left[n + \frac{t_{r(unknown)} - t_{r(n)}}{t_{r(N)} - t_{r(n)}} \right]$$

where:

I = Linear retention index

n = Number of carbon atoms in the n-alkane eluting immediately before the analyte

N = Number of carbon atoms in the n-alkane eluting immediately after the analyte

t_r = Retention time.

From the retention index, the absolute retention time was calculated using the retention times of n-alkanes as reference compounds.

These absolute retention times are not the original retention times used for the retention index calculation, but calculated values. This means that retention times can be calculated from the RIs present in an existing database using the locked retention times for n-alkanes if the column dimensions and the temperature program are the same[7].

This study analyzed several samples with no sample preparation. Only a few milligrams were introduced into the microvial (vial volume 40 µL). The selected samples were chosen because of their organoleptic properties, and because it was not possible to inject directly into the GC port using a syringe due to the complex matrix.

Results and discussion

Figures 1 and 2 show chromatograms with identified compounds and TICs of toothpaste, fabric softener, scented candle, and body lotion samples. Figure 3 shows the library search results from the MassHunter Unknowns Analysis software. Also, we can use the information from the Web to find out if the identified compound has a relationship with the flavor and fragrance industry (see Figure 4). If the message *Sorry, your search: "Docosyl octyl ether" returned zero results.* is displayed, this compound has no relationship with flavor or fragrance ingredients.

1,2. Hydrogen isocyanate
3. 3,5-Methanocyclopentapyrazole, 3,3a,4,5,6,6a-hexahydro-3a,4,4-trimethyl-
4. Phosphonic acid, (*p*-hydroxyphenyl)-
5. Eucalyptol
6. *gamma*-Terpinene
7. Linalol
8. Menthone
9. Cyclopentene, 1-isopropyl-4,5-dimethyl-
10. 1-Decene
11. 1-Decanol
12. Anethole
13. Eugenol
14. 7-Tetradecene, (Z)-
15. 1-Undecanol, acetate
16. Hydrogen isocyanate
17. Tetradecane, 1-chloro-
18. Lauryl alcohol
19. Pentadecane
20. *n*-Pentadecanol
21. 1-Nonadecene
22. Lauryl acetate
23. 1-Octadecanol
24. Sulfurous acid, butyl undecyl ester
25. 1-Docosene
26. Carbonic acid, hexadecyl prop-1-en-2-yl ester
27. *n*-Octadecane
28. Methoxyacetic acid, octadecyl ester
29. 1-Heneicosyl formate
30. 1-Hexacosene
31. Carbonic acid, eicosyl prop-1-en-2-yl ester
32. *n*-Eicosane
33. Disulfide, di-*tert*-dodecyl
34. 3,5,5-Trimethylhexyl ethylphosphonofluoridate
35. Docosyl octyl ether
36. 2-Ethylthiolane, S,S-dioxide
37. -[2,3-dihydro-4-hydroxy-2-(2-hydroxyisopropyl)benzofuran-7-yl]chromone
38. *n*-Tetracosane
39. Butyl triacontyl ether
40. Borane, diethyl(decyloxy)-
41. Aminomethanesulfonic acid
42. Ethyl-2methylbutyrate
43. Benzaldehyde
44. 3,7-Dimethyl-1-octanol
45. Octane, 4-chloro-
46. 1-Decanol
47. Cyclopropane, octyl-
48. 1-Dodecene
49. *gamma*-Nonalactone
50. 1-Tetradecene
51. Decyl acetate
52. 1H-Benzimidazole-2-carboxaldehyde
53. 2',4'-Dihydroxypropiophenone
54. Lauryl alcohol
55. Pentadecane
56. 1-Decanol, 2-hexyl-
57. 1-Hexadecanol
58. *n*-Hexadecane
59. Dodecyl heptyl ether
60. Isobutyl hexadecyl ether
61. 10-Heneicosene (c,t)
62. Oxalic acid, allyl tridecyl ester
63. Dodecyl nonyl ether
64. Trichloroacetic acid, pentadecyl ester
65. 1-Tricosene
66. Nonyl tetradecyl ether
67. Behenic alcohol
68. Carbonic acid, eicosyl vinyl ester
69. Silane, trichlorodocosyl-
70. *n*-Tetracosanol-1
71. *n*-Eicosane
72. Oxalic acid, cyclobutyl octadecyl ester
73. Docosyl pentyl ether
74. Isobutyl tetracosyl ether
75. Eicosyl octyl ether
76. Octacosyl trifluoroacetate
77. Hexacosyl pentyl ether

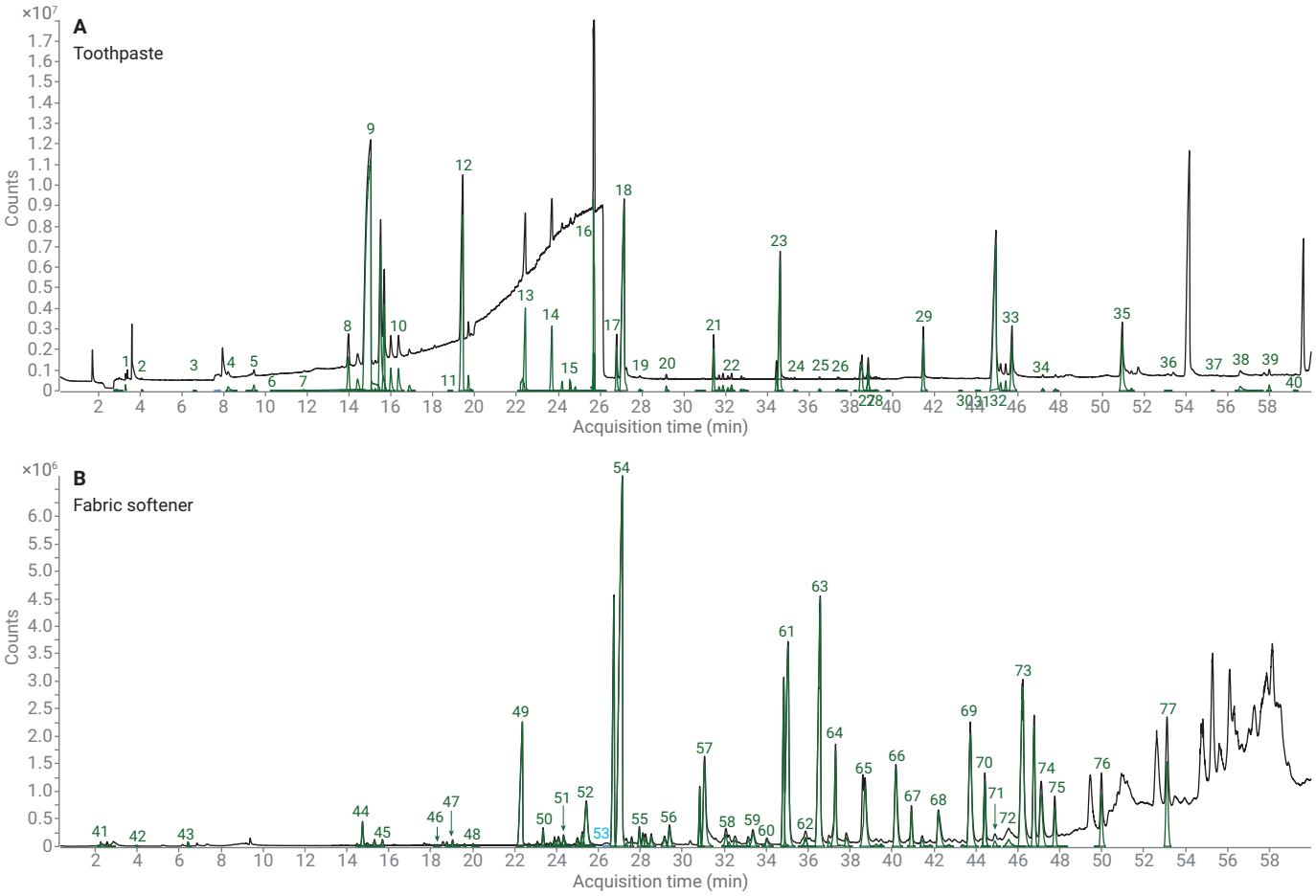


Figure 1. Toothpaste and fabric softener chromatograms showing identified compounds and TIC.

1. Nitrous oxide
2. Benzoyl isothiocyanate
3. 2,3-Heptadien-5-yne, 2,4-dimethyl-
4. Cyclohexane, 1-butenylidene-
5. *p*-Cresol
6. Methyl-1-silabenzocyclobutene
7. Methyl-1-silabenzocyclobutene
8. Citronellal
9. Menthone
10. L-Menthol
11. L-Menthol
12. *alpha*-Terpineol
13. Cyclopentane, 1-methyl-1-(2-methyl-2-propenyl)-
14. d-Piperitone
15. Benzofuran, 2-methyl-
16. Menthyl acetate; d,L-methyl-2-(methylethyl)cyclohexyl acetate
17. 2,4-Octadiene, 7,7-dimethyl-
18. Tridecane
19. Eugenol
20. *n*-Tetradecane
21. *beta*-Caryophyllene
22. 1H-Benzimidazole-2-carboxyaldehyde
23. 3,4-Dihydroxypropiophenone
24. 1-Hydroxy-7-hydroxymethylindane, cyclic sulfite ester
25. Propanoic acid, 2-methyl-3-[4-*t*-butyl]phenyl-
26. Isoamyl salicylate
27. *n*-Hexadecane
28. Fosfosal
29. Heneicosane
30. 1-Phenyl-2-(4-methylphenyl)-diazene 1-oxide
31. Benzyl benzoate
32. *n*-Octadecane
33. 2-Methylbenoic acid, 2-formyl-4,6-dichlorophenyl ester
34. Pentacosane
35. *n*-Eicosane
36. Sulfurous acid, octadecyl pentyl ester
37. Sulfurous acid, 2-ethylhexyl hexadecyl ester
38. Borane, diethyl(decyloxy)-
39. Hentriacontane
40. Dotriacontane
41. Tetracosane, 11-decyl-
42. Pentatriacontane
43. Arsenous acid, *tris*(trimethylsilyl) ester
44. Cyanogen bromide
45. 1,2-Propadiene-1,3-dione
46. 2,3,5-Trimethylpyrazine
47. 2-Propynenitrile, 3-fluoro-
48. 1-Hexene, 3,5-dimethyl-
49. Nonanal
50. 1-Pyrroline, 3-ethyl-
51. 3,7-Dimethyl-1-octanol
52. 1-Decene
53. 1-Decanol
54. 2-Propenal, 2-methyl-3-phenyl-
55. *gamma*-Nonalactone
56. Decyl acetate
57. Vanillin, isopropyl ether
58. Cinnamil acetate
59. 1-Tetradecanol
60. Ethanol, 2-(dodecyloxy)-
61. *n*-Pentadecanol
62. 1-Hexadecanol
63. Pentadecanoic acid
64. Octadecane, 1-isocyanato-
65. Hexadecane, 1,16-dichloro-
66. 10-Heneicosene (c,t)
67. Carbonic acid, pentadecyl prop-1-en-2-yl ester
68. Dodecyl nonyl ether
69. Dodecyl nonyl ether
70. 1-Eicosanol
71. Ethanol, 2-(octadecyloxy)-
72. Methoxyacetic acid, octadecyl ester
73. Octadecane, 1-isocyanato-
74. 1-Propanamine, 3-dibenzo[b,e]thiepin-11(6H)-ylidene-N,N-dimethyl-, S-oxide
75. Hexadecyl nonyl ether
76. 1-Hexacosene
77. Docosyl pentyl ether
78. 1-Propanamine, 3-dibenzo[b,e]thiepin-11(6H)-ylidene-N,N-dimethyl-, S-oxide
79. Carbonic acid, decyl hexadecyl ester
80. Docosyl octyl ether
81. 5H-Tetrazol-5-amine
82. 1-Propanamine, 3-dibenzo[b,e]thiepin-11(6H)-ylidene-N,N-dimethyl-, S-oxide
83. Chlorotrifluoromethane
84. Borane, diethyl(decyloxy)-

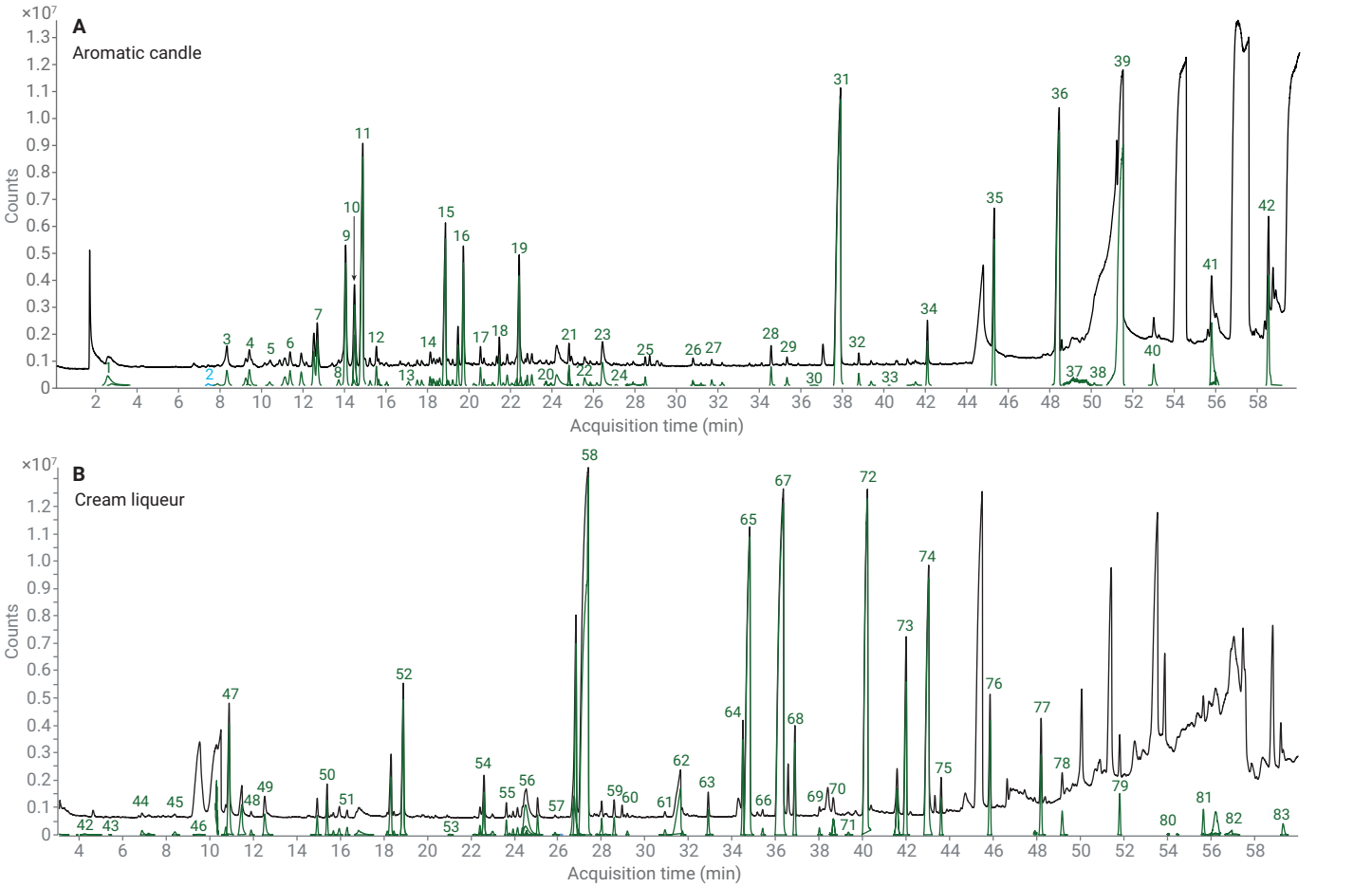
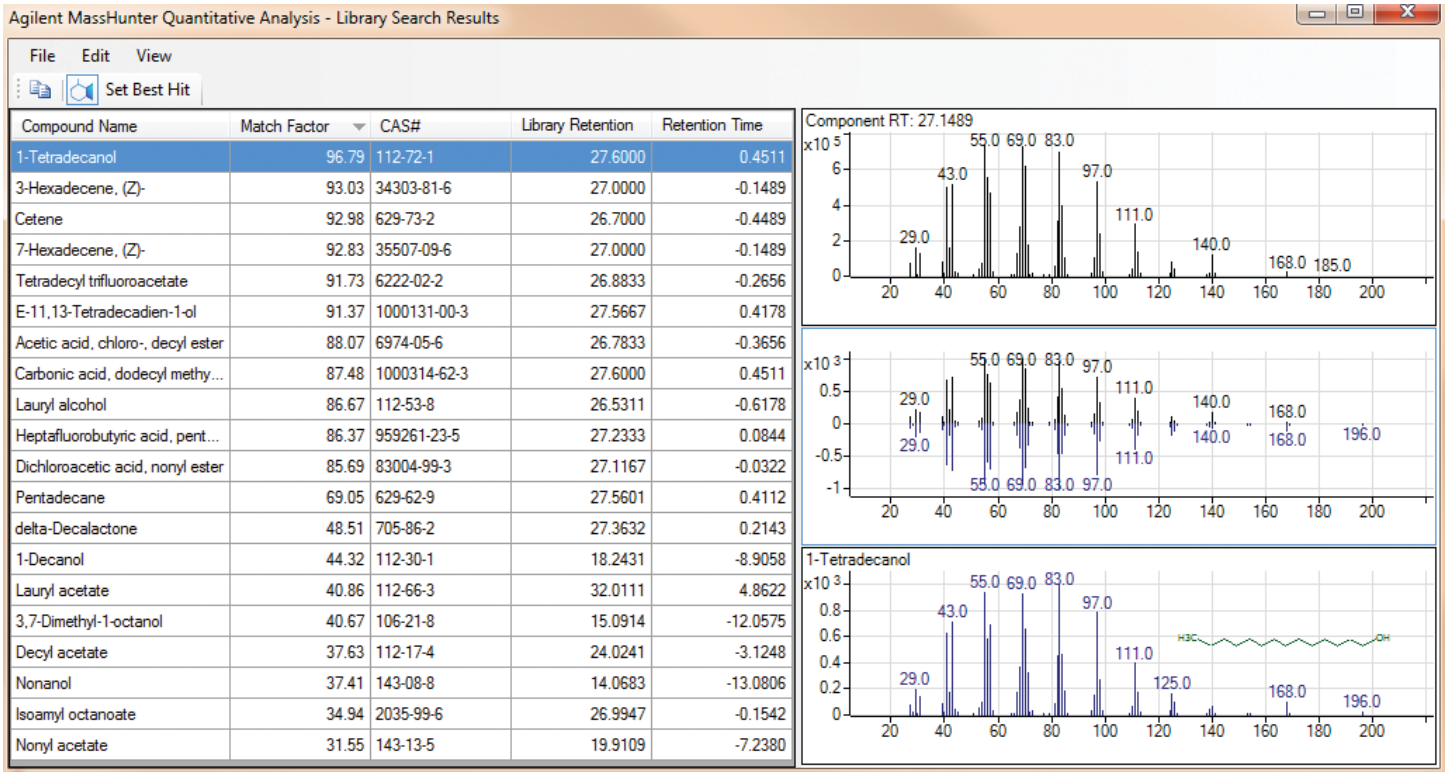


Figure 2. Scented candle and cream liqueur chromatograms showing identified compounds and TIC.



Compound Name	Match Factor	CAS#	Library Retention	Retention Time
1-Tetradecanol	96.79	112-72-1	27.6000	0.4511
3-Hexadecene, (Z)-	93.03	34303-81-6	27.0000	-0.1489
Cetene	92.98	629-73-2	26.7000	-0.4489
7-Hexadecene, (Z)-	92.83	35507-09-6	27.0000	-0.1489
Tetradecyl trifluoroacetate	91.73	6222-02-2	26.8833	-0.2656
E-11,13-Tetradecadien-1-ol	91.37	1000131-00-3	27.5667	0.4178
Acetic acid, chloro-, decyl ester	88.07	6974-05-6	26.7833	-0.3656
Carbonic acid, dodecyl methy...	87.48	1000314-62-3	27.6000	0.4511
Lauryl alcohol	86.67	112-53-8	26.5311	-0.6178
Heptafluorobutyric acid, pent...	86.37	959261-23-5	27.2333	0.0844
Dichloroacetic acid, nonyl ester	85.69	83004-99-3	27.1167	-0.0322
Pentadecane	69.05	629-62-9	27.5601	0.4112
delta-Decalactone	48.51	705-86-2	27.3632	0.2143
1-Decanol	44.32	112-30-1	18.2431	-8.9058
Lauryl acetate	40.86	112-66-3	32.0111	4.8622
3,7-Dimethyl-1-octanol	40.67	106-21-8	15.0914	-12.0575
Decyl acetate	37.63	112-17-4	24.0241	-3.1248
Nonanol	37.41	143-08-8	14.0683	-13.0806
Isoamyl octanoate	34.94	2035-99-6	26.9947	-0.1542
Nonyl acetate	31.55	143-13-5	19.9109	-7.2380

Figure 3. MassHunter Unknowns Analysis software enables the evaluation of an alternative using the match factor and retention time. This information can be sorted by the match factor or by the retention time difference between the component RT and the library RT.

eugenol
4-allyl-1-hydroxy-2-methoxybenzene

Cosmetic Information:

CosIng: cosmetic data

Cosmetic Uses: denaturants, perfuming agents, tonic

stearyl alcohol
1-hydroxyoctadecane

Cosmetic Information:

CosIng: cosmetic data

Cosmetic Uses: emollients, emulsifying agents, emulsion stabilisers, foam boosting agents, masking agents, opacifying agents, refatting agents, surfactants, viscosity controlling agents

Figure 4. Information about eugenol and stearyl alcohol obtained from the Web, and the hyperlink was used to created a MassHunter Unknown Analysis.

Components

Compound Name	CAS#	Match Factor	Library File	Component RI	Delta RI	Library RI	Component RT	Delta RT	Library RT
Linalol	78-70-6	83.9	flavor_RI_NoR...	1101	0	1101	11.8274	-0.0088	11.8186
Isopulegol	59905-53-2	84.4	flavor_RI_NoR...	1146	-2	1144	13.6518	-0.0676	13.5842
l-Menthone	14073-97-3	98.5	NIST17.L	1154	-6	1148	13.9649	-0.8293	13.1355
Menthone	14073-97-3	85.8	flavor_RI_NoR...	1165	-1	1164	14.4009	-0.0446	14.3563
L-Menthol	2616-51-5	91.7	flavor_RI_NoR...	1186	-12	1173	15.2483	-0.5016	14.7467
Cyclopentane, 1-butyl-2-propyl-	62199-50-2	94.8	NIST17.L	1192	27	1219	15.5049	0.5188	16.0237
Methylsalicylate	119-36-8	98.0	flavor_RI_NoR...	1197	-3	1194	15.6796	-0.1025	15.5771
4-Undecene, 5-methyl-, (Z)-	74630-69-6	92.7	NIST17.L	1204	-5	1199	15.9913	-0.7845	15.2068
Cyclopentane, 1-butyl-2-propyl-	62199-50-2	91.4	NIST17.L	1213	6	1219	16.3576	-0.3339	16.0237
Cyclopentane, 1-hexyl-3-methyl-	61142-68-5	92.9	NIST17.L	1226	-7	1219	16.8742	-0.8505	16.0237
Spiro[5.5]undecane	180-43-8	80.3	NIST17.L	1240	-6	1234	17.4660	-0.8190	16.6470
1-Decanol	112-30-1	86.4	flavor_RI_NoR...	1272	0	1272	18.8128	-0.0031	18.8097
trans-Anethole	4180-23-8	99.1	flavor_RI_NoR...	1288	-2	1285	19.4354	-0.0962	19.3392
(-)-Neomenthylacetate	1000152-81-2	93.2	NIST17.L	1294	10	1304	19.7039	-0.1485	19.5553

Figure 5. Analysis of the toothpaste sample. Some components were identified by the Agilent library, others were identified by NIST17. In both cases, the system calculates the retention time using the retention index from the libraries. Also, there are two hyperlinks: the hyperlink for the CAS number goes to the NIST webpage to get chemical information, and the hyperlink for the compound name goes to the Good Scents company webpage to get information about organoleptic and cosmetic properties, suppliers, safety data sheet, and so on.

Components

Compound Name	CAS#	Match Factor	Library File	Component RI	Delta RI	Library RI	Component RT	Delta RT	Library RT
Lauryl alcohol	112-53-8	98.7	flavor_RI_NoR...	1477	-3	1474	27.1406	-0.1049	27.0357
Lauryl alcohol	112-53-8	94.9	flavor_RI_NoR...	1575	-101	1474	31.0604	-4.0247	27.0357
Lauryl alcohol	112-53-8	91.7	flavor_RI_NoR...	1429	45	1474	25.2327	1.8030	27.0357
Lauryl alcohol	112-53-8	84.7	flavor_RI_NoR...	1752	-278	1474	37.3101	-10.2744	27.0357
Lauryl alcohol	112-53-8	90.0	flavor_RI_NoR...	1533	-59	1474	29.3837	-2.3480	27.0357
Lauryl alcohol	112-53-8	92.3	flavor_RI_NoR...	1488	-14	1474	27.5848	-0.5491	27.0357
Lauryl alcohol	112-53-8	95.4	flavor_RI_NoR...	1686	-212	1474	35.0377	-8.0020	27.0357
Lauryl alcohol	112-53-8	95.4	flavor_RI_NoR...	1383	92	1474	23.3611	3.6746	27.0357
Lauryl alcohol	112-53-8	90.6	flavor_RI_NoR...	1638	-164	1474	33.3644	-6.3287	27.0357
Lauryl alcohol	112-53-8	86.4	flavor_RI_NoR...	1528	-53	1474	29.1545	-2.1188	27.0357

Figure 6. In this table, the RT match penalty was disabled, resulting in lauryl alcohol being detected 10 times, all of them with a match factor over 84. But only one has the lower delta RT and the highest match factor. This feature made compound identification easier. When this feature was enabled, only one compound appeared in the search results.

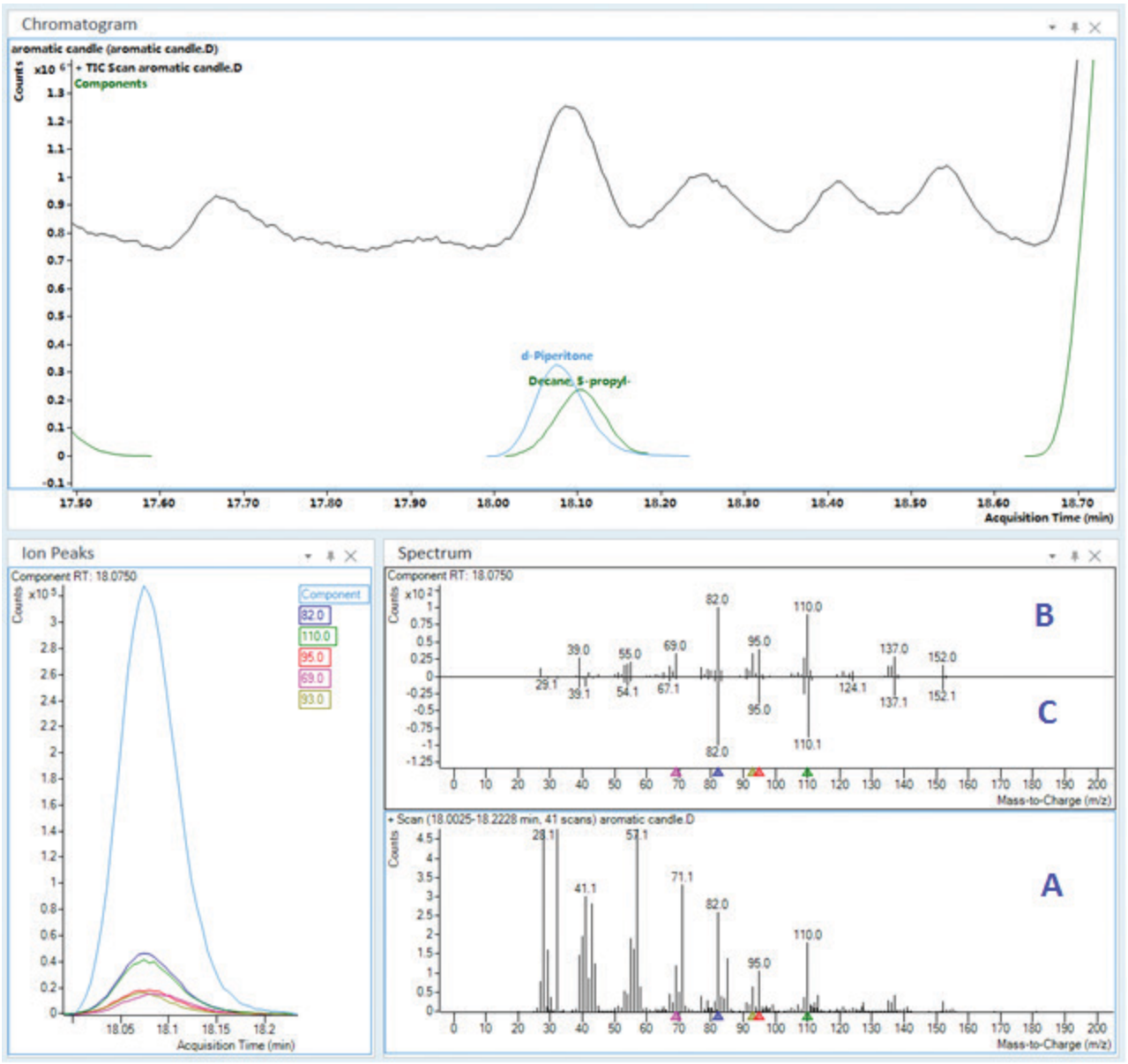


Figure 7. MassHunter Unknowns Analysis software uses a deconvolution algorithm to separate two coeluting compounds. The undeconvoluted spectrum (A), compound deconvoluted spectrum (B), and library spectrum (C) are displayed in the same window to make data review easier.

Conclusions

A method was developed for the analysis of flavors and fragrances in complex matrices without sample preparation. A small quantity of sample was deposited into the microvial, and inserted in the inlet port. The method may be used for quality control analysis. The method is retention-time-locked using n-hexadecane as the locking standard. A retention index database, containing approximately 400 compounds, was modified from an existing method. This database can be used to identify constituents based on their absolute retention time under the locked conditions. The locked method also guarantees retention time stability as a function of time, between columns, and between instruments.

Finally, it is shown that RIs for flavor compounds measured under specific operational conditions can be transferred into locked retention times using the locked retention times of n-alkanes. Thus, existing RI databases can be translated into locked retention time databases.

References

1. Tabacchi, R.; Garnero, J. *Capillary Gas Chromatography in Essential Oil Analysis*; Sandra, P., Bicchi, C., Eds.; Huthig: Heidelberg, **1987**; 1–11.
2. Jennings, W.; Shibamoto, T. *Qualitative Analysis of Flavor and Fragrance Volatiles by Glass Capillary Gas Chromatography*; Academic Press: New York, **1980**.
3. Shibamoto, T. *Capillary Gas Chromatography in Essential Oil Analysis*; Sandra, P., Bicchi, C., Eds.; Huthig: Heidelberg, **1987**; 259–274.
4. Adams, R. P. *Identification of Essential Oil Components by Gas Chromatography - Mass Spectroscopy*; Allured Publishing Corporation: IL, USA, **1995**.
5. Ping, X.; Menge, C.-K.; Zslewski, M. Building Agilent GC/MSD Deconvolution Reporting Libraries for Any Aplication, *Agilent Technologies Technical Overview*, publication number 5989-2249EN, **2005**.
6. David, F. *et al.* Analysis of Essential Oil Compounds Using Retention Time Locked Methods and Retention Time Databases, *Agilent Technologies Application Note*, publication number 5988-6530EN, **2002**.
7. Sandy, C.; Butler, I. Incorporating Retention Index Results in Deconvoluted GC/MS Library Search Data, *Agilent Technologies Data Sheet*, publication number 5991-8221EN, **2017**.
8. Giarrocco, V.; Quimby, B.; Klee, M. Retention Time Locking: Concepts and Applications, *Agilent Technologies Application Note*, publication number 5966-2469E, **1997**.

Appendix

Figure 8 shows the workflow for creating deconvoluted GC/MS libraries with LRI values, and processing sample data files in MassHunter Unknowns Analysis software. The full procedure can be found in the Agilent Technologies Data Sheet *Incorporating Retention Index Results in Deconvoluted GC/MS Library Search Data*, publication number 5991-8221EN.

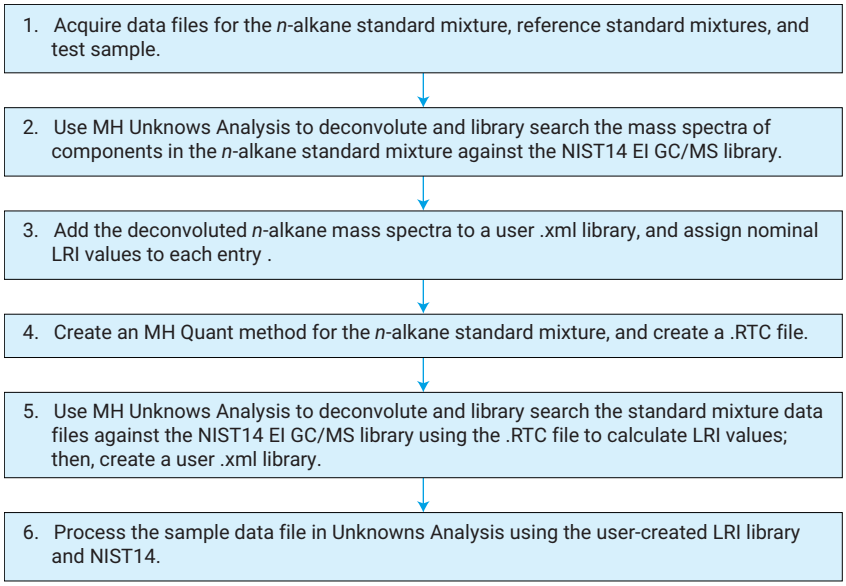


Figure 8. Workflow for creating deconvoluted GC/MS libraries with LRI values.

To provide qualitative information on the components of complex flavor and fragrance mixtures, user libraries can be searched in combination with commercially available GC/MS libraries (such as NIST17). Deploying retention time locking or linear RIs can improve confidence in analyte identification by reducing false positives. Mass spectral deconvolution provides better quality mass spectra of closely eluting/overlapping components when searching in GC/MS libraries.

To get more information about a selected compound, a hyperlink can be created in MassHunter Unknowns Analysis software.

1. Open the *QuantAnalysis.exe.config* file in the path: *ProgramFiles\Agilent\MassHunter\Workstation\Quant\bin* and edit the link to the desired URL. This file is read-only by default, so you need to disable this feature.
2. Open the file, and look for the line: *<add key="Column.CASNumber.Action" value="URL:http://webbook.nist.gov/cgi/cbook.cgi?ID={0}"/>.*
3. Add the next line to create the new hyperlink into MassHunter for the compound name *<add key="Column.CompoundName.Action" value="URL:http://www.thegoodscentscompany.com/search3.php?qName={0}"/>.*
4. Save the file.
5. Start MassHunter Unknowns Analysis software. Now, you have a new hyperlink in the compound name field that connects with the Web to get organoleptic and cosmetic information, data sheet, and so on (Figures 9 and 10).

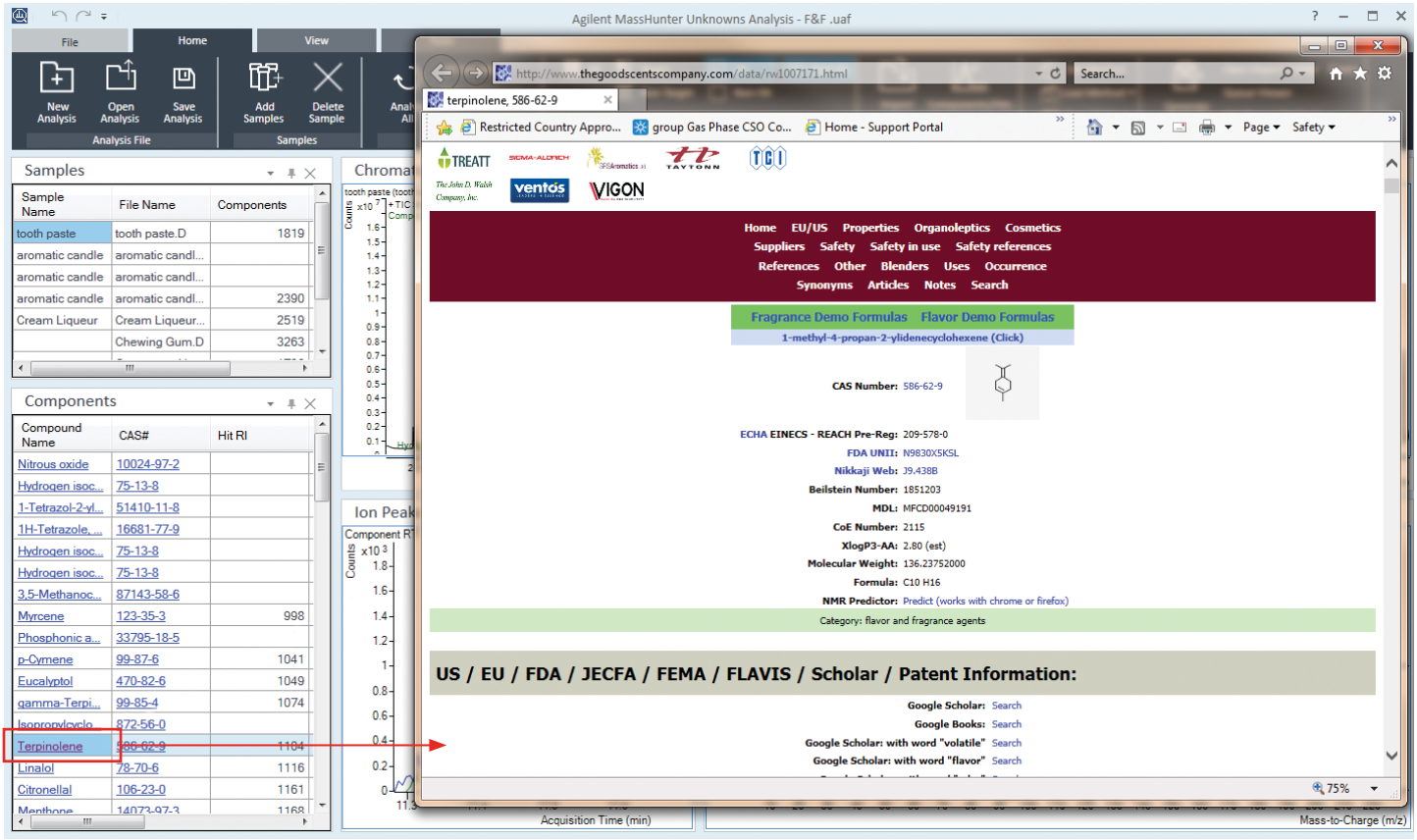


Figure 9. Hyperlink connecting a compound name to a web page, in MassHunter Unknowns Analysis software.

Home EU/US Properties Organoleptics Cosmetics
Suppliers Safety Safety in use Safety references
References Other Blenders Uses Occurrence
Synonyms Articles Notes Search

Fragrance Demo Formulas Flavor Demo Formulas

1-methyl-4-propan-2-ylidenecyclohexene (Click)

CAS Number: 586-62-9

ECHA EINECS - REACH Pre-Reg: 209-578-0
FDA UNII: N9830X5KSL
Nikkaji Web: J9.438B
Beilstein Number: 1851203
MDL: MFCD00049191
CoE Number: 2115
XlogP3-AA: 2.80 (est)
Molecular Weight: 136.23752000
Formula: C10 H16
NMR Predictor: Predict (works with chrome or firefox)

Category: flavor and fragrance agents

FDA Regulation:

FDA PART 172 -- FOOD ADDITIVES PERMITTED FOR DIRECT ADDITION TO FOOD FOR HUMAN CONSUMPTION
Subpart F--Flavoring Agents and Related Substances
Sec. 172.515 Synthetic flavoring substances and adjuvants.

Physical Properties:

Appearance: colorless clear liquid (est)
Assay: 95.00 to 100.00 %
Food Chemicals Codex Listed: No
Specific Gravity: 0.88000 to 0.89000 @ 25.00 °C.
Pounds per Gallon - (est).: 7.322 to 7.406
Refractive Index: 1.46000 to 1.46400 @ 20.00 °C.
Boiling Point: 183.00 to 185.00 °C. @ 760.00 mm Hg
Vapor Pressure: 1.126000 mm/Hg @ 25.00 °C. (est)
Vapor Density: 4.7 (Air = 1)
Flash Point: 148.00 °F. TCC (64.44 °C.)
logP (o/w): 4.470
Shelf Life: 24.00 month(s) or longer if stored properly.
Storage: store in cool, dry place in tightly sealed containers, protected from heat and lig

Soluble in:

alcohol
water, 9.5 mg/L @ 23C (exp)

Stability:

alcoholic fine fragrance, fair
antiperspirant, good
deo stick
fabric softener, good
hard surface cleaner
liquid detergent, good
perborate powder detergent, poor
shampoo
soap, good

Figure 10. Example of compound information from an associated webpage (http://www.thegoodscentscompany.com).

www.agilent.com/chem

This information is subject to change without notice.

© Agilent Technologies, Inc. 2019
Printed in the USA, April 11, 2019
5994-0546EN

Agilent
Trusted Answers