



## Rapid Qualitative GC/TOFMS Analysis of Peppermint Oil

Peppermint oil is one of the most extensively used essential oils, both medicinally and commercially. It is an important ingredient in a variety of consumer products ranging from candy to nausea remedies. Minor variations in peppermint oils from different sources can significantly alter the flavor and ultimately the quality of a product. Consequently, careful analysis of peppermint oil components is important to ensure the manufacture of uniform products over time.

Gas chromatography (GC) with flame ionization detection (FID) is commonly used to characterize peppermint oil. However, these analyses are lengthy requiring 45 minutes or more to allow complete chromatographic resolution of the individual components for identification.

Alternately, analyses of peppermint oil extracts with fast GC techniques and the LECO Pegasus II Time-of-Flight Mass Spectrometer (TOFMS) are complete in less than 2 minutes. Fast acquisition rates (up to 500 spectra per second) allow for unique and automated spectral deconvolution of overlapping chromatographic peaks. The resulting mass spectra coupled with retention indices are used to identify individual components.

General GC/TOFMS conditions were established for a variety of essential oil extracts. These general conditions, outlined below, were used without further optimization to analyze a sample of peppermint oil.<sup>1</sup> The total acquisition time for the analysis was less than 2 minutes. Automated data processing and library searching against both the NIST and Terpene Essential Oil<sup>2</sup> mass spectral databases resulted in 73 identified components.

**Table 1:** GC and TOFMS Conditions for a 2 Minute Analysis of Peppermint Oil.

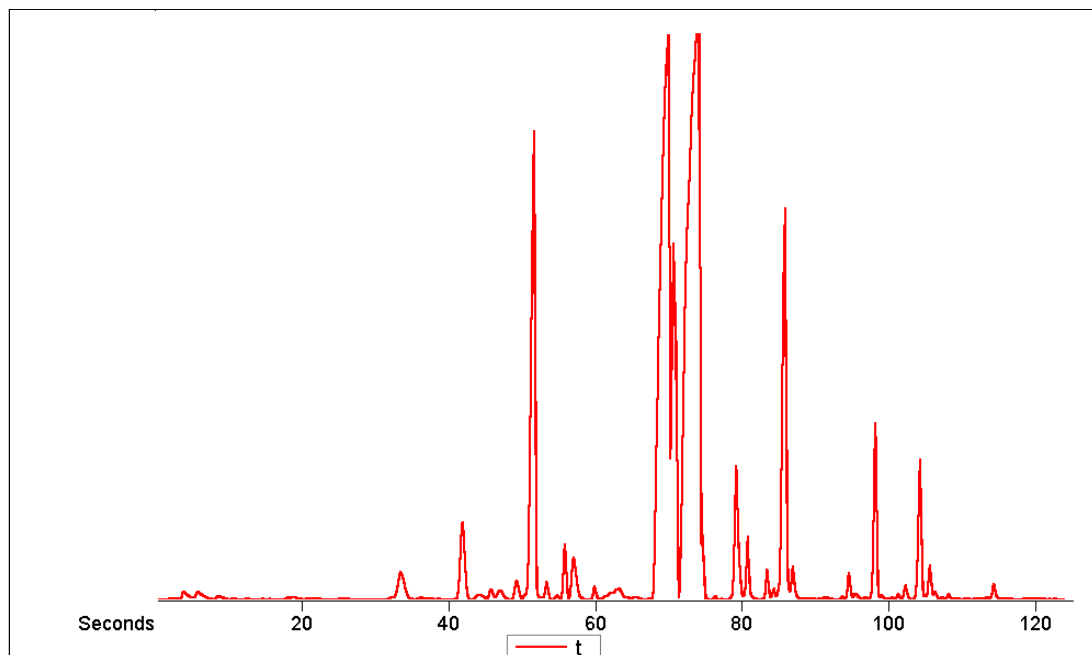
Detector:	LECO Corporation Pegasus II Time-of-Flight Mass Spectrometer
Transfer Line:	300°C
Source:	200°C
Acquisition Rate:	30 spectra/sec (35 to 400 u)
GC:	Hewlett Packard® 6890*
Column:	DB-5 4 m x 0.1 mm ID, 0.1µm phase film
Oven:	40°C for 0.5 min., then to 280°C at 75°C/min., hold for 1 min.
Injector:	290°C
Carrier Gas:	Helium, 2.0 ml/min. constant flow
Sample:	No preparation required. 0.1 µL split (200:1) injection.

\*HP6890 GC is equipped with fast oven temperature ramp capabilities and a high pressure EPC module.

<sup>1</sup>Thanks to Kathleen K. Webb and A.M. Todd Company for providing a sample of peppermint oil and helping with analyte identification.

<sup>2</sup>Robert P. Adams. *Identification of Essential Oil Components by Gas Chromatography/Mass Spectroscopy*. Allured Publishing Corporation, Carol Stream, IL. 1995.

**Figure 1:** Total Ion Chromatogram (TIC) for a 1.9 Minute Analysis of Peppermint Oil.



**Table 2:** Compound Name, Retention Time (RT), Library Hit Number and Spectral Similarity Index for Essential Oil Reference Standard Analysis.

Peak	Name	RT (sec)	Hit Number	Similarity
1	Propanal, 2-methyl-	4.31	1	881
2	1-Propanol, 2-methyl-	5.26	1	695
3	Butanal, 3-methyl-	5.76	3	729
4	Butanal, 2-methyl-	5.96	1	885
5	Furan, 2-ethyl-	7.06	1	838
6	1-Butanol, 3-methyl-	8.66	1	865
7	2-Hexenal	18.16	1	857
8	3-Hexen-1-ol	19.06	1	845
9	trans-2-Hexen-1-ol	20.86	1	768
10	1-Hexanol	21.36	1	818
11	Furan, 2,5-diethyltetrahydro-	25.66	1	827
12	$\alpha$ -Pinene	33.51	7	874
13	$\beta$ -Pinene	41.91	1	921
14	1-Octen-3-ol	44.11	2	882
15	$\beta$ -Myrcene	45.81	1	883
16	3-Octanol	46.91	1	880
17	$\alpha$ -Phellandrene	47.16	1	794
18	$\alpha$ -Terpinene	49.31	2	861
19	o-Cymene*	50.56	1	861
20	Limonene	51.61	1	783
21	Eucalyptol	51.71	1	866
22	Benzeneacetaldehyde	53.06	1	834
23	Cis- $\beta$ -ocimene	53.41	1	904
24	trans- $\beta$ -Ocimene*	54.81	1	874
25	$\gamma$ -Terpinene	55.86	2	855
26	cis-Sabinene Hydrate*	57.06	4	791
27	cis-Linalool Oxide	57.86	1	743
28	Terpinolene	59.91	2	888
29	2-Methylbutyl 2-methylbutanoate	62.81	1	886
30	Linalool	63.06	2	845
31	Pentyl 3-methylbutanoate	63.46	1	906
32	1,7-Octadien-3-ol, acetate	64.21	1	644

Peak	Name	RT (sec)	Hit Number	Similarity
33	Acetic acid, 1-ethylhexyl ester	65.96	1	741
34	Menthone	69.21	1	912
35	Menthofuran	70.46	1	827
36	Isomenthone	70.71	2	882
37	Neo-Menthol	71.06	2	916
38	4-Terpineol	72.26	1	723
39	Menthol	73.61	6	906
40	$\alpha$ -Terpineol	74.71	1	751
41	Myrtenol	75.26	2	611
42	trans-Piperitol	76.36	1	728
43	Pulegone	79.26	1	923
44	Carvone	79.66	1	902
45	Carvacrol, Methyl Ether-*	79.81	2	770
46	Hexyl n-valerate	80.06	1	743
47	p-Anisaldehyde	80.41	1	775
48	Piperitone	80.81	1	885
49	Neomenthyl acetate	83.41	2	858
50	2H-1-Benzopyran, 3,4,4a,5,6,8a-hexahydro-2,5,5,8a-tetramethyl-, (2 $\alpha$ ,4 $\alpha$ ,8 $\alpha$ )-	84.36	1	825
51	Dihydroedulan I	84.91	1	818
52	Menthyl acetate	85.86	3	895
53	Isomenthyl acetate	86.96	1	900
54	Benzenemethanol, 3,5-dimethyl-	87.31	1	656
55	cis-Pinocarvyl Acetate*	88.56	3	685
56	cis-Verbenyl Acetate*	91.21	1	726
57	Eugenol	91.71	5	782
58	Copaene	93.76	1	852
59	$\beta$ -Bourbonene	94.61	1	882
60	$\beta$ -Elemene*	95.51	1	785

Peak	Name	RT (sec)	Hit Number	Similarity
61	$\alpha$ -trans-Bergamotene*	96.81	2	720
62	9-epi-trans-Caryophyllene*	98.16	4	881
63	Germacrene D*	99.06	6	752
64	cis- $\gamma$ -Cadinene*	100.51	1	784
65	$\alpha$ -Humulene	101.31	1	860
66	trans- $\beta$ -Farnesene*	102.31	4	814

Peak	Name	RT (sec)	Hit Number	Similarity
67	$\gamma$ -Muuroolene*	104.31	1	831
68	Bicyclogermacrene*	105.66	1	888
69	Germacrene A*	106.36	3	817
70	$\gamma$ -Cadinene*	107.31	2	764
71	$\delta$ -Cadinene*	108.21	2	810
72	Caryophyllene Oxide*	113.36	1	816
73	Globulol*	114.31	2	811

\*Library match from the Essential Oil database. All other matches are from the NIST database.

Ninety percent of the components in the reference standard are correctly identified in the top three library hits. For those analytes where the correct library match is further down the hit list, the preceding hits are structural isomers of the correct analyte.

### Conclusions:

The LECO Pegasus II GC/TOFMS system reduces data collection time by more than 1 order of magnitude. This fast acquisition coupled with automated data processing results in greater sample turnover and increased productivity.



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