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Application News
GCMS

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Rapid Analysis of Bergamot Oil and Patchouli Oil by Fast GC/MS

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An essential oil is a liquid extract of the volatile aromatic compounds from plants. Essential oils are used in perfumery, aromatherapy, cosmetics, medicine, as well as in flavoring in food and drink. As part of the quality assurance practice in fragrance analysis, the compositions of essential oils often need to be determined. In this case, specificity and analysis time are two important factors in quality assurance.

Fast gas chromatography mass spectrometry (GC/MS) technique offers an increased specificity of the results as well as reduced analysis time. Through a comparison of the retention indices and the mass spectra the compounds in an essential oil can be identified. Comparison of mass spectra can be performed against general mass spectral a library or special flavor/fragrance mass spectral libraries. Analysis times, which usually range from 30 minutes to 60 minutes, can be reduced drastically without sacrificing the specificity.

Here we report Fast GC/MS analysis of two essential oils bergamot oil and patchouli oil where the analysis time is reduced to about 4 and 6 minutes, respectively. This 5-fold reduction of analysis time can significantly increase sample throughput and reduce the cost per analysis.

GC/MS Method

Selection of parameters used for fast GC/MS analysis and for conventional GC/MS analysis are shown in Table 1 and Table 2, respectively.

Table 1. Fast GC/MS

GC/MS	Shimadzu GCMS-QP2010 + AOC-20i auto-injector
Injection volume	0.2 µL
Injector	Split/splitless
Injector temperature	280°C
Injection mode	Split, split ratio = 800:1
Carrier gas	Helium
Flow control mode	Constant Linear Velocity
Linear velocity	60 cm/s
Column inlet pressure	421.5 kPa @ 40°C
Column	Rtx-5, 10 m x 0.10 mm i.d. x 0.10 µm (Restek Corp.)
Column oven program	40°C (0 min) - 30°C/min - 300°C
Interface temperature	280°C
Ionization	Electron Impact
Mass range	40 – 500 a.m.u.
Scan interval	0.1 sec

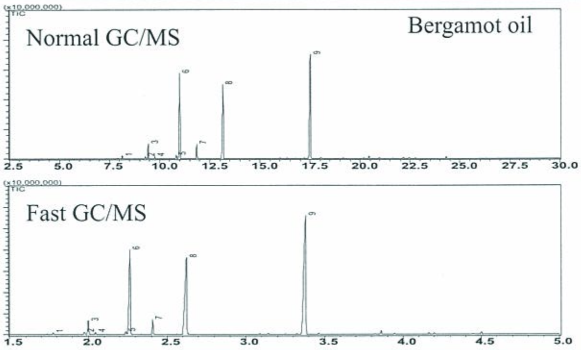
Table 2. Conventional GC/MS

GC/MS	Shimadzu GCMS-QP2010 + AOC-20i auto-injector
Injection volume	1.0 µL
Injector	Split/splitless
Injector temperature	280°C
Injection mode	Split, split ratio = 100:1
Carrier gas	Helium
Flow control mode	Constant Linear Velocity
Linear velocity	36 cm/s
Column inlet pressure	46.7 kPa @ 40°C
Column	Rtx-5SilMS, 30 m x 0.25 mm i.d. x 0.25 µm (Restek Corp.)
Column oven program	40°C (0.5 min) - 5°C/min - 300°C
Interface temperature	280°C
Ionization	Electron Impact
Mass range	40 – 500 a.m.u.
Scan interval	0.4 sec

Results

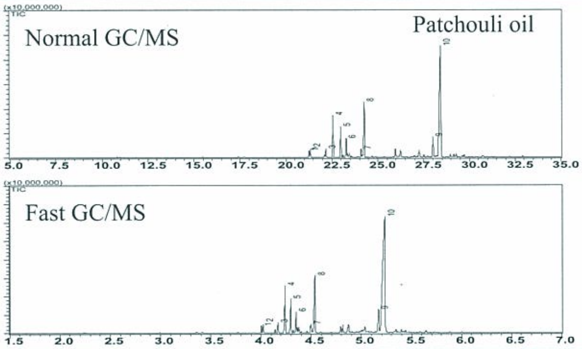
In fast GC/MS, capillary columns with significantly shorter length and smaller diameters are used. This gives rise to two important requirements for the GC/MS system. First, higher column inlet pressures are required for the GC (typically 400 - 900 kPa) to deliver the necessary carrier gas linear velocity. Second, the peaks width obtained in fast GC/MS are generally smaller (sharper) than those obtained in normal GC/MS analysis; this requires a high scan rate (data acquisition rate) by the MS system (5000 a.m.u./sec or higher) in order to obtain good quality mass spectra for accurate identification of the peaks. A standard GCMS-QP2010 is able to meet these two requirements.

Figures 1 and 2 demonstrate the reduction in analysis time when analyzing bergamot oil and patchouli oil, respectively, by using fast GC/MS. In normal GC/MS, a 5°C/min column temperature gradient and a carrier gas linear velocity of 36 cm/s were necessary to achieve good resolution of the peaks. In fast GC/MS, we could use a 30°C/min column temperature gradient and a carrier gas linear velocity of 60 cm/s and still achieved a good resolution. Figures 3 and 4 show the details of some critical separations in bergamot oil and patchouli oil analysis.



1. alpha-Pinene
2. Sabinene
3. beta-Pinene
4. beta-Myrcene
5. p-Cymene
6. D-limonene
7. gamma-Terpinene
8. Linalol
9. Linalyl acetate (bergamol)

Figure 1. Total Ion Chromatogram of bergamot oil analysis by normal and fast GC/MS.



1. beta-Patchoulene
2. beta-Elemene
3. Caryophyllene
4. alpha-Guaiene
5. Seychellene
6. alpha-Patchoulene
7. Guaiene
8. delta-Guaiene
9. Selinene
10. Patchouli alcohol

Figure 2. Total Ion Chromatogram of patchouli oil analysis by normal and fast GC/MS.

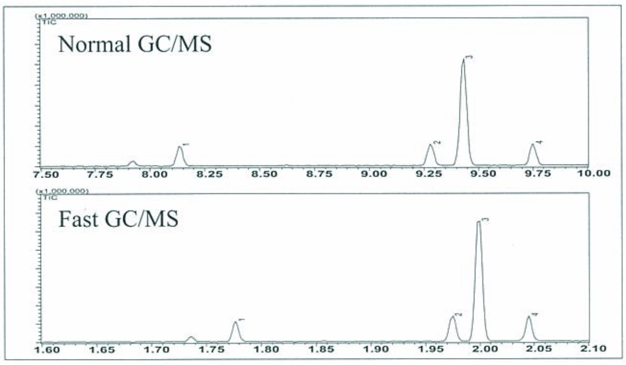


Figure 3. Details of critical separations in bergamot oil analysis by normal and fast GC/MS.

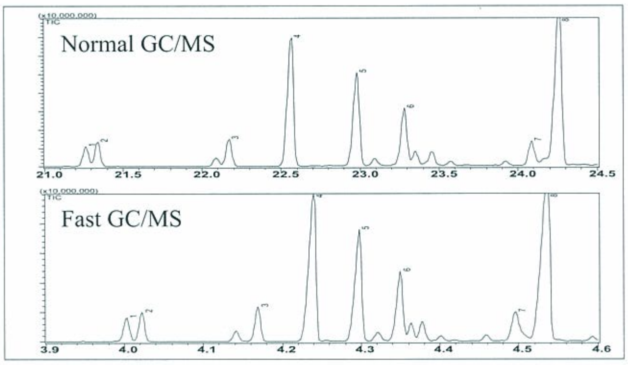


Figure 4. Details of critical separations in patchouli oil analysis by normal and fast GC/MS.

Conclusion

Analysis times can be reduced drastically without significant loss of separation efficiency when fast GC/MS technique is used. Small diameter and short capillary columns are required to achieve a good separation in a much shorter analysis time. High GC column inlet pressure is necessary to guarantee optimum carrier gas linear velocity for the analysis. Fast MS scan (data acquisition) rates are also required in order to obtain good quality mass spectra for library search and sufficient number of scans for a peak for good peak integration. Both of these instrument parameters are standard features in GCMS-QP2010.

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