NOTE

Deconvolution of Overlapping GC-MS Peaks in Rose Essential Oil: A Comparison Study between ChemoPower and Agilent Masshunter

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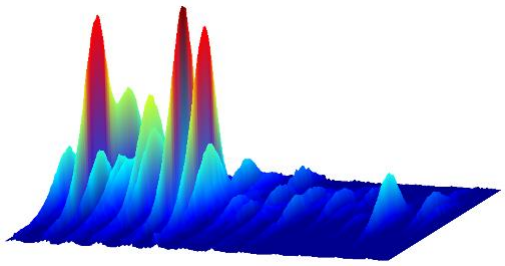
Abstract



GC-MS is a vital analytical instrument for analytical labs. The complication of overlapping peaks is a major problem for analysis of complex herb mixtures. The development of algorithms to deconvolute and reconstruct pure component signals has thus provided a convenient approach to identify individual components and reconstruct pure spectra from complex mixtures. The performance of ChemoPower's algorithm will be compared against Agilent Masshunter software for the analysis of rose essential oil in this note.

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Background

The analysis of herb mixtures with gas chromatography-mass spectrometry (GC-MS) is often complicated by the occurrence of overlapping peaks due to co-eluting components. While experimental modifications could potentially separate the overlapping peaks, it is a time and labor intensive process. The need for software deconvolution to identify components in overlapping peaks is thus essential for complex GC-MS total ion chromatogram (TIC) profiles. Several softwares have been developed over the years to support the deconvolution analysis of complex TIC profiles including AMDIS, Agilent Masshunter, MZMine 2 etc. The various softwares apply different nature of algorithms which thus provide varying degree of accuracy in deconvoluting overlapping GC-MS peaks.

ChemoPower has developed a proprietary deconvolution algorithm to provide qualitative and quantitative analyses on overlapping GC-MS peaks. The algorithm is based on the Entropy Minimization approach. On the other hand, Agilent has recently introduced Masshunter software which supports deconvolution of overlapping peaks based on their proprietary deconvolution algorithm. In this note, the performance of ChemoPower's algorithm is compared against Agilent Masshunter software for the analysis of known and *unknown* components in herb mixtures.

This study is based on the TIC profile of rose essential oil. The TIC profile obtained from an Agilent GC-MS system is shown in **Figure 1** with the inset focusing on the TIC time from 1624 to 1716 seconds. The TIC intervals of interest for analysis are labeled as A and B, which are both highly overlapping peaks.

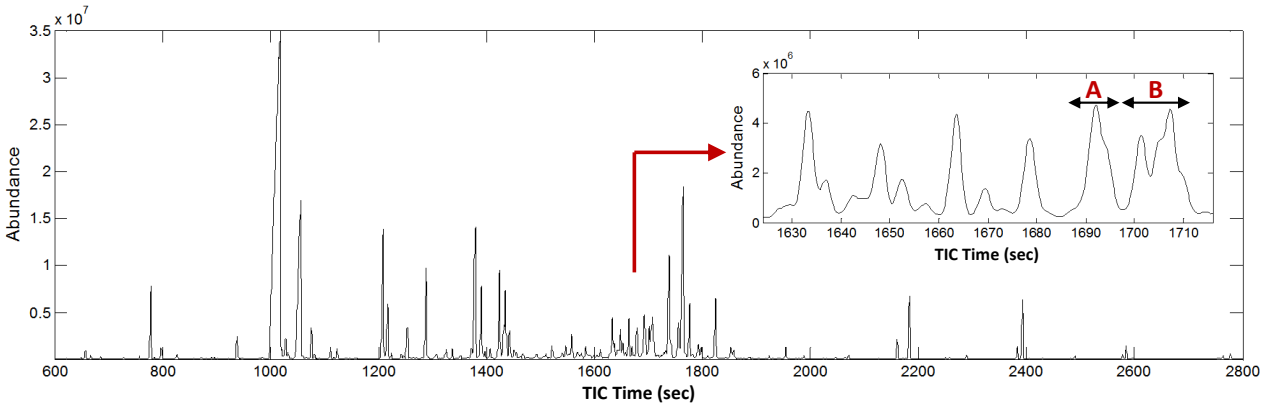

Figure 1. Total ion flow chart of rose essential oil sample. Inset: Interval of 1624–1712 seconds. TIC profile obtained from Agilent GC-MS 7890A-5975C system under electron ionization mode at 70 eV and full-scan mode.

Deconvolution with ChemoPower's algorithm

ChemoPower's entropy minimization algorithm was applied on intervals A and B to deconvolute the TIC profile and mass spectra as shown in **Figure 2a-b**. Intuitively, intervals A and B should contain two and four components, respectively. In fact, ChemoPower's algorithm was able to reconstruct four components for each interval of A and B (labeled A1-4 and B1-4). The ratios of estimated TIC profile to real TIC profile were 95.8 % and 99.4 % for intervals A and B, respectively. Since the estimated TIC profile were very similar to the real TIC profile, further quantitative analysis on the co-eluted peaks *via* existing methods (external/internal standards) could be further performed. In addition, the peak width of approximately 5 seconds for each deconvoluted components was comparable to typical peaks of pure components under normal GC-MS analysis. More importantly, the deconvolution capability of ChemoPower's algorithm could reveal interesting details on overlapping peaks, for example, the overlapping peak shoulders of components B1 and B4 at approximately 1707 seconds. Careful analysis of the deconvoluted spectra showed a high degree of overlap across numerous m/z positions. This could imply the possible presence of isomers or homologues in the rose essential oil. On top of that, the good estimated TIC profile allows for subsequent accurate quantitative analysis to determine the percentage composition of the isomers or homologues.

Deconvolution with Agilent Masshunter

The analysis was subsequently performed on Agilent Masshunter Qualitative Analysis software as shown in **Figure 2c**. For interval A, only one deconvoluted component (labeled A1') was obtained while for interval B, three deconvoluted components (labeled B1'-3') were identified. The estimated TIC profile did not coincide with the real TIC profile as a result of the poor deconvolution. In fact, the abundance of estimated TIC profile of interval A was lower than the real TIC profile while that of interval B exceeded the real TIC profile. Moreover, the peak widths of the deconvoluted components were rather huge at approximately 8 seconds. On closer observation at B1' and B3', they were deconvoluted as two-peak components due to a high degree of overlap across numerous m/z positions in the deconvoluted spectra. This would greatly reduce any possibilities of identifying or quantifying potential isomers or homologues. The abrupt termination of the bases of both peaks before plateauing off also contributed to the lower accuracy of the deconvolution.

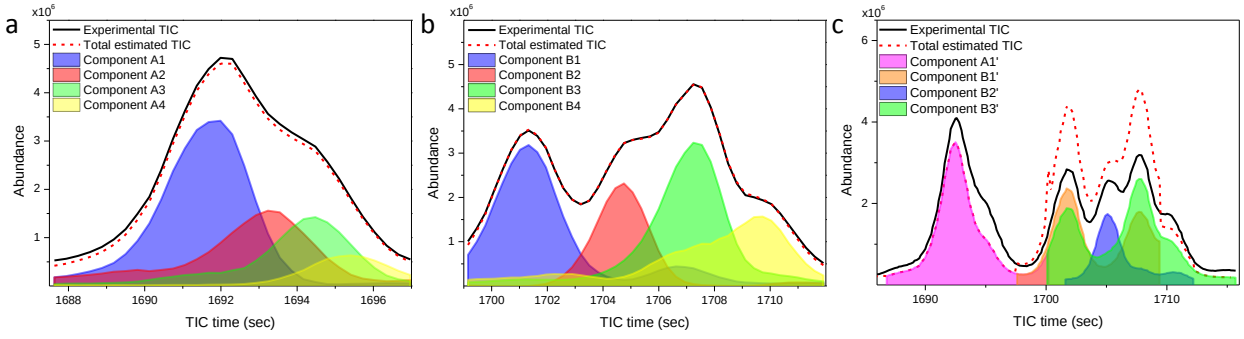

Figure 2. ChemoPower's deconvolution of TIC profile for intervals (a) A and (b) B. Interval A was 1687–1697 seconds while interval B was 1698–1712 seconds. (c) Agilent Masshunter deconvolution of TIC profile for intervals A and B. Performed under default "find by chromatogram deconvolution" settings of Agilent Masshunter Qualitative Analysis software version B.06.00.

Discussions

The deconvoluted components were matched against the 2014 NIST mass spectral library and the analyses are shown in **Table 1**. At first glance, both ChemoPower's algorithm and Agilent Masshunter software were able to identify the presence of α-bisabolol (A1 and A1'), 2-pentadecanone (B2 and B2') and trans-farnesol (B3 and B3') at comparatively similar TIC time and R.Match value. However, the matching analysis of ChemoPower's algorithm returned a higher NIST Probability value, which could potentially assist the analyst in making better judgments. The Probability value for component B3' was particularly low at only 8.8 %.

For the case of interval A, ChemoPower's algorithm was able to identify the presence of 2,3-dihydrofarnesol (A3) at a good R.Match and high Probability values. On the other hand, Agilent Masshunter was able to provide only one deconvoluted component despite the obvious peak shoulder observed at TIC time of 1695 sec. For the case of interval B, Agilent Masshunter identified the presence of aristolone (B1') with fair R.Match value but very low Probability value. However, the retention index of 1746 for aristolone which deviated from the retention index trend suggested a possible false positive detection.

On another note, the components A2, A4, B1 and B4 identified by ChemoPower's algorithm were *unknown* compounds since no suitable (poor Match, R.Match and Probability values) NIST matching was achieved. Nevertheless, the deconvoluted spectra of the known *unknowns* could be recorded for future use with the upcoming release of ChemoPower's algorithm for the structural identification of unknown compounds.

Table 1. Matching analysis of the deconvoluted components and spectra against 2014 NIST mass spectral library.

Components	TIC time (sec)	Chemical Name	Retention index (i.u.)	Formula	NIST R.Match	NIST Prob. (%)
ChemoPower						
A1	1692.0	α-Bisabolol	1665 (est. 1621)	$C_{15}H_{26}O$	916	83.3
A3	1694.5	2,3-Dihydrofarnesol	est. 1661	$C_{15}H_{28}O$	833	74.2
B2	1704.8	2-Pentadecanone	1682	$C_{15}H_{30}O$	827	55.1
B3	1707.2	trans-Farnesol	1690	$C_{15}H_{26}O$	827	55.6
Agilent Masshunter						
A1'	1692.5	α-Bisabolol	1665	$C_{15}H_{26}O$	938	69.4
B1'	1701.8	Aristolone	1746	$C_{15}H_{22}O$	789	16.2
B2'	1705.0	2-Pentadecanone	1682	$C_{15}H_{30}O$	799	52.1
B3'	1707.8	trans-Farnesol	1690	$C_{15}H_{26}O$	829	8.8

Conclusion

In summary, the deconvolution performance of ChemoPower's algorithm was compared against Agilent Masshunter for the GC-MS analysis of highly overlapping peaks in rose essential oil. ChemoPower's algorithm was able to identify a total of eight components from two sets of overlapping peaks while Agilent Masshunter could identify only four components. The estimated TIC profile obtained from ChemoPower's algorithm overlapped the real TIC profile at a high accuracy while Agilent Masshunter provided either underestimated or overestimated TIC profiles. In addition, four components with relatively high R.Match and Probability values were identified by ChemoPower's algorithm while Agilent Masshunter only managed two components of similar matching scores. While not included in this short technical note, ChemoPower's algorithm is also able to provide quantitative analysis (in terms of %) for the deconvoluted components since the estimated TIC profile is very similar to the real TIC profile.

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