Case Studies brochure

ChemoPower

Cutting Edge Innovation

in Mass Spectral Analysis

Empower Your Research

The Power of Chemometrics!
ChemoPower
Singapore

Saving You Valuable Resources……

…Whatever Your Discipline

One of the major challenges for accurate GC-MS and LC-MS analysis is to achieve excellent chromatographic separation with high signal-to-noise ratio. However, real-world samples are often contaminated with impurities that manifest as background noise or peaks. The occurrence of overlapping peaks due to coeluting components further complicates the analysis. In fact, these complications can be easily resolved with data analysis software. As such, having a state-of-the-art hardware without the most competent data analysis software to decipher complicated data is a big waste of resources.

ChemoPower's proprietary peak deconvolution software – SmartDalton™ – provides a unique solution to analyze complicated GC-MS and LC-MS data. Incorporated with an advanced algorithm capable of resolving overlapping peaks and spectra with high background noise, SmartDalton™ delivers accurate qualitative and quantitative analysis even for severely coeluting and trace-level components. The robustness of the system simplifies and revolutionizes the application of GC-MS and LC-MS analysis, saving you valuable time and resources.

The Power of Chemometrics!
ChemoPower
Singapore

Core Technology

Proprietary algorithm for the analysis of GC-MS and LC-MS data:

- Automated peak deconvolution based on entropy minimization

Key Innovation in GC-MS and LC-MS

ChemoPower's unique solution for GC-MS and LC-MS data analysis is proven to provide fast and accurate qualitative and quantitative results, without the need for any prior information on the analyte. Regardless of peak intensity or coelution complications, ChemoPower delivers accurate results consistently and even identify unknown components in complex matrices.

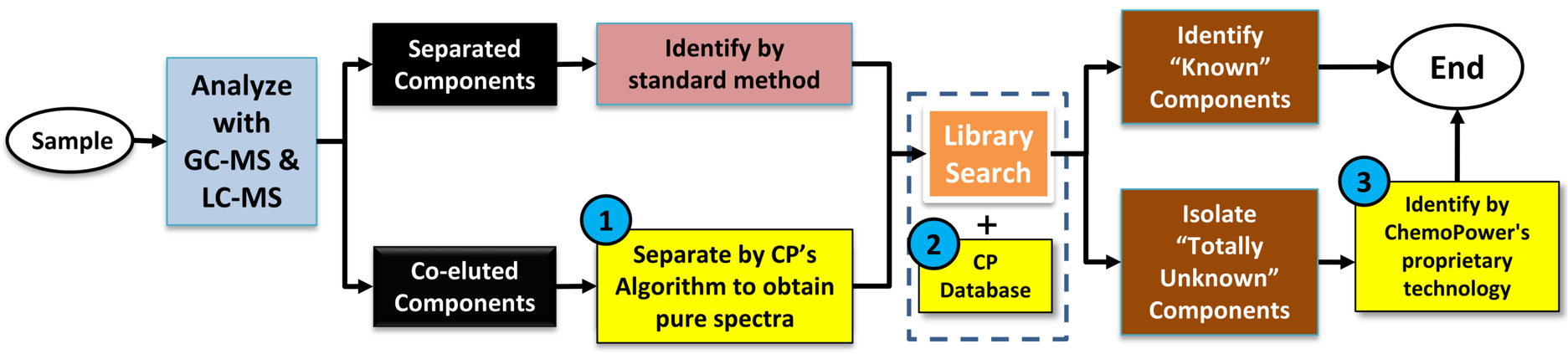
Patented Technology SmartDalton™

SmartDalton™ is a desktop client software that incorporates ChemoPower's proprietary peak deconvolution technology.

SmartDalton™ delivers:

- Superior automated batch data processing and component identification capabilities
- Seamless integration to custom mass spectral libraries
- Mass spectral reader (CDF, mzXML, mzML, and mzData)
- Mass spectral export capability for manual screening
- Integral reporting function which provides user-customizable report templates
- Additional customization as required

ChemoPower's Unique Full Analysis Solution



Competitive Advantages

Time Savings
Digitally separate compounds in mixtures up to 100 times faster. This replaces the hours spent in the laboratory tuning the equipment to physically separate the compounds.

Enhanced Capabilities
Identify unknown components in mixtures without any prior information on the analyte, which existing conventional methods are not capable of.

Simplified Process
Reduce manpower required by simplifying and automating analysis process such that results are obtained by a few clicks of the mouse.

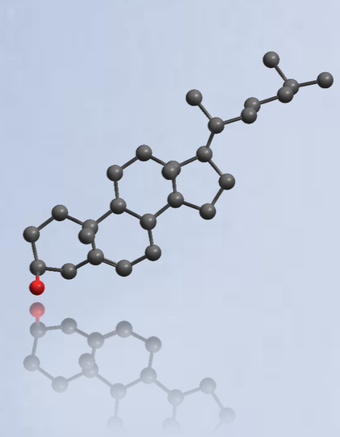
Universal Compatibility
ChemoPower's unique software works well with data collected from all major equipment vendors

Available Online
Software is online allowing access and usage anytime and anywhere.

Cost Savings
ChemoPower's solution requires only inexpensive equipment with basic functions, which lead to lower consumables and running cost. There is no requirement of highly skilled professionals to operate.

Data Analysis

Case Studies



Resolves Complex Coeluting peaks With Confidence

Case 1 Deconvolution of Overlapping GC-MS Peaks in Rose Essential Oil

Background

Essential oils are known to contain hundreds of chemical compounds. The GC-MS analysis of essential oils is usually complicated by the presence of overlapping peaks due to coeluting components. In order to achieve physical separation of the overlapping peaks, extensive experimental modifications that are both time and labor intensive have to be performed.

ChemoPower's proprietary peak deconvolution software – SmartDalton™ – is capable of resolving complex overlapping peaks to provide accurate qualitative and quantitative analysis. The pure mass spectra of coeluting components are automatically extracted regardless of whether they are unknown or known components.

This study is to clearly highlight the strength and accuracy of SmartDalton™ in finding, identifying and quantifying coeluted components, as compared to Agilent Masshunter.

Scope

A TIC profile of rose essential oil is examined in this case study. The TIC profile is shown in **Figure 1** with the inset focusing on a region containing numerous overlapping peaks. The TIC intervals of interest for analysis are labeled as A and B, which are both severely overlapping peaks.

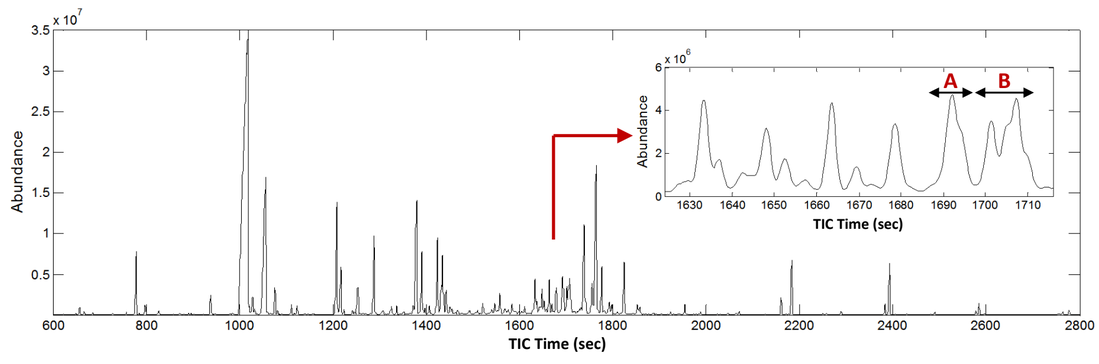


Figure 1. Total ion chromatogram of rose essential oil sample collected with Agilent GC-MS 7890A-5975C.

Deconvolution with SmartDalton™

SmartDalton™ deconvoluted intervals A and B to reconstruct four components for each interval (labeled A1-4 and B1-4), as shown in Figure 2a-b. The deconvolution was accurate since similar number of components was observed on the surface plots of the raw GC-MS data (Figure 2d). Furthermore, the ratios of estimated TIC to experimental TIC were 95.8 % and 99.4 % for intervals A and B, respectively.

Deconvolution with Masshunter

Masshunter Qualitative Analysis software provided one deconvoluted component (labeled A1') for interval A and three deconvoluted components (labeled B1'-3') for interval B (Figure 2c). As a result of poor deconvolution, the component profiles were distorted and the estimated TIC profile did not coincide with the experimental TIC profile.

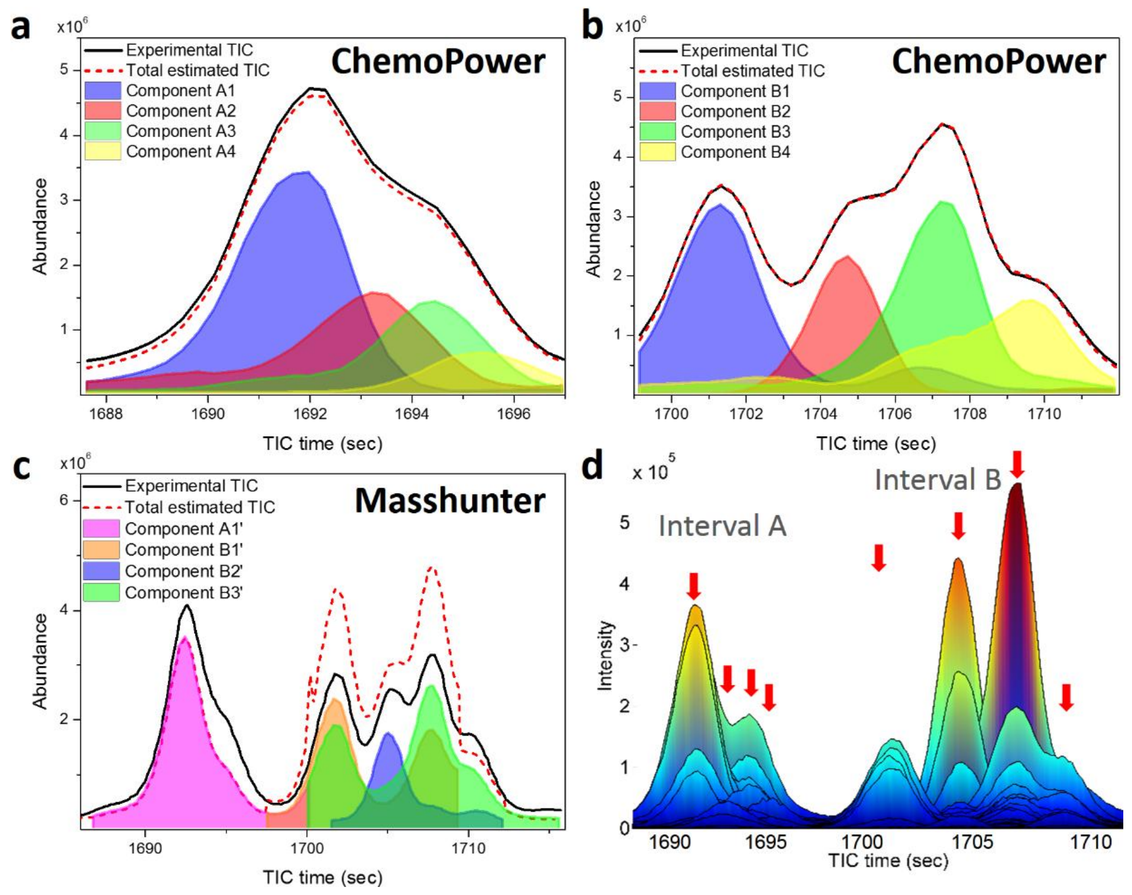


Figure 2. Deconvolution results from (a-b) ChemoPower and (c) Masshunter. (d) Surface plot of raw GC-MS data for Interval A and B

Conclusion

SmartDalton™ identified a total of four components from two sets of overlapping peaks while Masshunter identified only three components. The library match results are shown in Table 1. The pure component spectra extracted by SmartDaltonTM returned higher match probability values than Masshunter, which would assist the analyst in making better judgments.

Components A2, A4, B1 and B4 identified by SmartDalton™ were unknown compounds since no suitable library matches were achieved. The pure mass spectra of these known *unknowns* could be recorded for future analysis.

Table 1. Library match analysis of the deconvoluted component spectra against NIST 2014 mass spectral library.

Components	TIC time (sec)	Chemical Name	Retention index	Formula	Reverse Match	Probability (%)
SmartDalton™						
A1	1692.0	α-Bisabolol	1684	$C_{15}H_{26}O$	916	83.3
A3	1694.5	2,3-Dihydrofarnesol	1696	$C_{15}H_{28}O$	833	74.2
B2	1704.8	2-Pentadecanone	1698	$C_{15}H_{30}O$	827	55.1
B3	1707.2	trans-Farnesol	1697	$C_{15}H_{26}O$	827	55.6
Masshunter						
A1'	1692.5	α-Bisabolol	1684	$C_{15}H_{26}O$	938	69.4
B2'	1705.0	2-Pentadecanone	1698	$C_{15}H_{30}O$	799	52.1
B3'	1707.8	trans-Farnesol	1697	$C_{15}H_{26}O$	829	8.8

SmartDalton™ was also able to provide quantitative analysis (in terms of area percentage) for the deconvoluted components since the estimated TIC profile was very similar to the experimental TIC profile.

Case 2 Qualitative and Quantitative Analyses of Overlapping GC-MS Peaks

Background

The development of GC-MS hardware has hit a plateau in recent years and much focus has shifted to the development of data processing software instead. The robustness of the data processing software resides mainly on the accuracy of its peak analysis capability. To be more specific, the software should accurately deconvolute and reconstruct pure component spectra from complex TIC data to provide qualitative and quantitative analysis.

This study is to highlight the deconvolution performance of SmartDalton™ and compare against that of AMDIS and Masshunter in a controlled mixture sample consisting of four unique components – methanol, dichloromethane, acetonitrile and 1,4-dioxane.

Scope

This study differentiates the deconvolution performances using a controlled mixture sample. Equal volumes of the said chemicals are mixed to form the controlled mixture sample. The GC-MS settings were modified to ensure the coelution of the four chemical components. Next, another GC-MS settings were used to separate the four components in order to obtain their peak areas (read as Real values). The deconvolution analysis with ChemoPower's SmartDalton™, Masshunter and AMDIS were performed on the overlapping peaks of the controlled mixture.

Analysis with SmartDalton™

SmartDalton™ deconvoluted and reconstructed four pure component spectra and they were matched against the 2014 NIST spectral library. Excellent reverse match (> 850) and probability (> 78 %) values were obtained from the analysis and correctly correlated to the four chemicals. The area percentages for the components were also closely similar to the Real values. Moreover, the ratio of the total estimated TIC to experimental TIC was 99.4 % and the inner product value was 1.000, indicating accurate deconvolution.

Analysis with Masshunter

Masshunter deconvolution result provided four pure components spectra leading to the correct identification of the four chemicals. However, the TIC profiles of methanol and 1,4-dioxane consisted of two peak apexes as a result of inaccurate deconvolution. As such, the area percentages for the components differ from that of the Real values and thus resulted in an inaccurate quantitative analysis.

Table 1. Comparison of retention time and area percentage analysis of real results against ChemoPower, Masshunter and AMDIS.

Component	Retention Time, sec				Area Percentage, %		
	Real	ChemoPower	Masshunter	AMDIS*	Real	ChemoPower	Masshunter
Methanol	141.24	140.65	140.70	140.76	11.05	12.5	16.1
Dichloromethane	141.78	142.02	142.02	141.30 141.90 142.02 142.62	40.29	39.3	42.3
Acetonitrile	142.80	143.40	143.40	143.40 144.12	19.39	18.1	17.1
1,4-Dioxane	144.36	144.54	144.48	143.88 144.48 144.60	29.27	30.1	24.5

*AMDIS computed multiple positions for the same component.

Analysis with AMDIS

AMDIS analysis resulted in the detection of 11 peaks corresponding to five unique components. On top of the four expected chemicals, AMDIS shortlisted N,N-dimethylacetamide as a possible component. This constituted as a false positive.

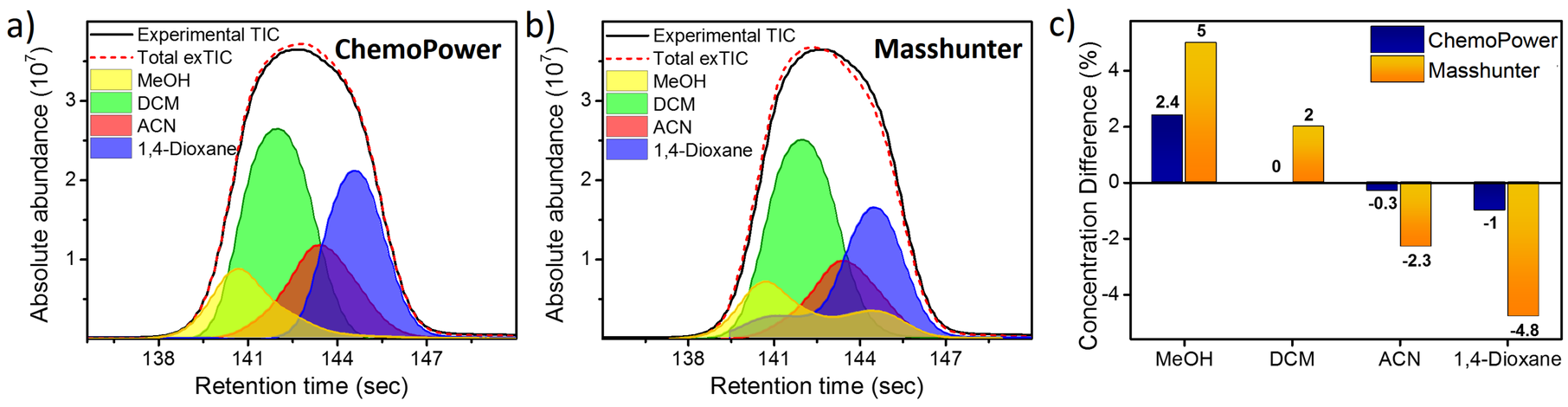


Figure 1. Deconvolution results from (a) ChemoPower and (b) Masshunter. (c) Bar plot showing the deviations of ChemoPower and Masshunter quantitative analysis with comparison from Real values.

Conclusion

The performance of SmartDalton™ to obtain accurate qualitative and quantitative analysis was compared against that of AMDIS and Masshunter by analyzing a co-eluted GC-MS TIC profile consisted of methanol, dichloromethane, acetonitrile and 1,4-dioxane. In terms of qualitative analysis SmartDalton™ and Masshunter provided accurate results while AMDIS reported a false positive result. In terms of quantitative analysis based on area percentage, Masshunter suffered from high percentage errors (5 - 46 %) while SmartDalton™ provided a more accurate (2 – 13 %) results. Apart from the accuracy of SmartDalton™, the entire analysis process is automated as no user-dependent settings or a priori information is required.

Case 3 Comprehensive Metabolite Profiling of Eucalyptus exserta

Background

Comprehensive profiling of complex mixtures such as essential oils is highly challenging due to the presence of numerous trace and co-eluted chemical compounds. Despite the availability of various data processing software, they do not always provide accurate and confident identification and annotation of chemical components.

This study shows the clear advantage of SmartDalton™ against Masshunter in providing comprehensive untargeted profiling for an essential oil of Eucalyptus exserta..

Scope

A TIC profile of Eucalyptus essential oil is examined in this case study. The TIC profile is shown in Figure 1. All the components in the TIC profile were analyzed in detail to provide both qualitative and quantitative analysis. The tentative identification and annotation of the components were supported by usage of retention indices.

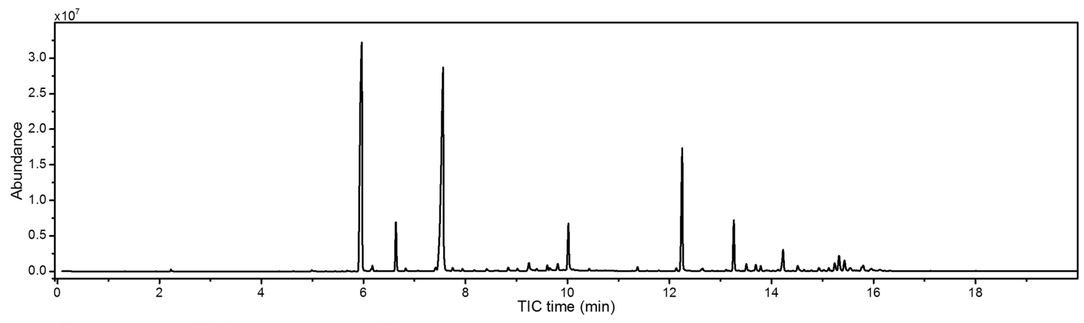


Figure 1. TIC profile of Eucalyptus exserta.

Analysis with SmartDalton™

Chemopower's SmartDalton™ reconstructed the pure spectra for 134 components, in which 122 components were identified and the remaining 12 components were unknown (Figure 2). On the basis of retention index, 112 components were tentatively annotated.

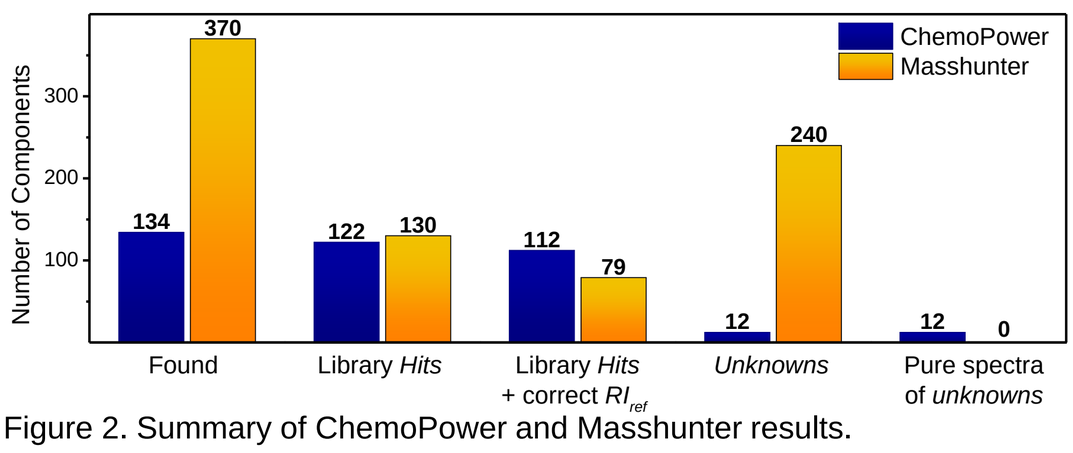


Figure 2. Summary of ChemoPower and Masshunter results.

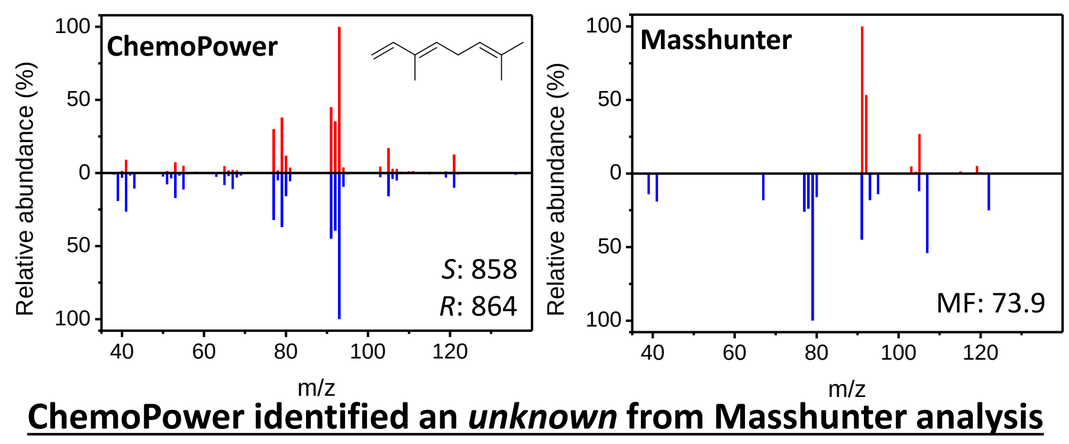
Analysis with Masshunter

Masshunter found 370 components, in which 130 components were identified and 240 components were unknown (Figure 2). Based on the retention index, only 79 components were tentatively annotated. In fact, most of the unknown components corresponded to results that were either duplicates or false positives. As such, it is challenging or almost impossible for Masshunter to provide accurate identification and annotation of components.

The analysis of components 34 and 101 would provide a clear comparison between the performance of SmartDalton™ and Masshunter. Overall, SmartDalton™ extracted purer component spectra than Masshunter to enable accurate tentative annotation of components (Figure 3). The reconstructed spectrum of component 34 by SmartDalton™ led to the confident identification of (E)-β-Ocimene at high match scores (S and R > 800). However, the spectrum provided by Masshunter failed to provide accurate identification. Subsequent analysis on component 101 by SmartDalton™ led to the identification of viridiflorene with excellent match scores. However, Masshunter identified the component as an unknown. Masshunter is not able to reconstruct pure spectra accurate, thus leading to erroneous analysis.

ChemoPower extracts purer spectra than Masshunter

Component 34 at t_R = 7.58 min – (E)-β-Ocimene



ChemoPower identified an *unknown* from Masshunter analysis

Component 101 at t_R = 14.20 min – Viridiflorene

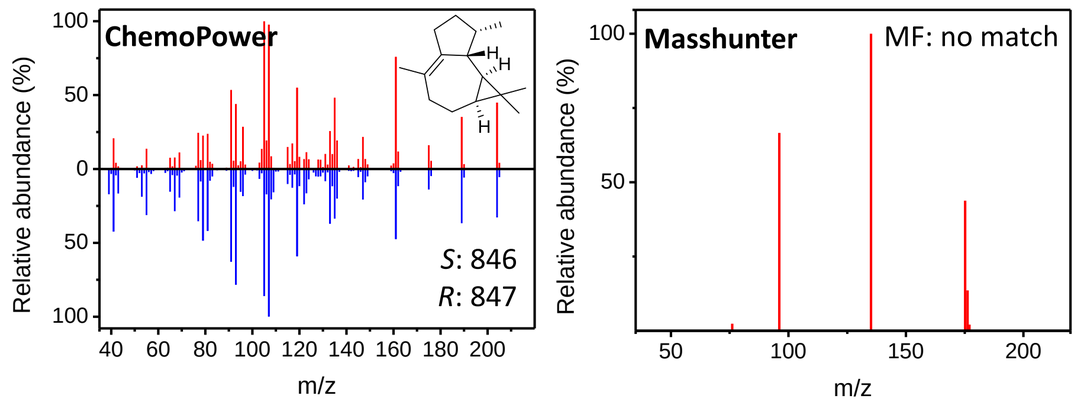


Figure 3. Comparison of ChemoPower and Masshunter results on components 34 and 101.

Conclusion

Mass spectral deconvolution is fundamentally important for comprehensive untargeted profiling by GC-MS. The inaccurate reconstruction of spectra can potentially lead to misleading results. ChemoPower's spectral deconvolution algorithm SmartDalton™ introduces a new approach to achieve accurate and confident untargeted profiling for GC-MS data.

SmartDalton™ provides an indiscriminative nature of analysis whereby the presence and mass spectra of both known and unknown components can be determined. With SmartDalton™, 112 components were tentatively identified, which was in excess of 42 % when compared to Masshunter. SmartDalton™ has outperformed Masshunter in terms of both accuracy and confidence of analysis.

Delivers Accurate
Results without
Compromise

Case Studies

Case 4 Deconvolution of Overlapping Peaks in GC-MS analysis of Rhizoma Chuanxiong herb

Background

Herbs contain a plethora of volatile chemical compounds that give rise to their unique aromas or flavors. It is extremely challenging to determine each and every compound due to the sheer amount of compounds present and the vast quantity of coeluted peaks. This poses a complicated problem for analysts to identify the compounds.

In such cases, modifying the experimental procedures, such as the sample preparation protocols, GC-MS parameters and parts are often time-consuming and costly. ChemoPower's SmartDalton™ is capable of providing accurate qualitative and qualitative results without modifications as well as user's input of parameter settings.

This study is to highlight the deconvolution performance of SmartDalton™ on GC-MS analysis of Rhizoma Chuanxiong herb, compared against that of AMDIS and Masshunter.

Scope

The performance of SmartDalton™ would be compared to both AMDIS and Agilent Masshunter software based on the analysis of a co-eluted peak in a sample of Rhizoma Chuanxiong herb. The TIC profile is shown in Figure 1 and the area of interest for deconvolution is highlighted in the inset.

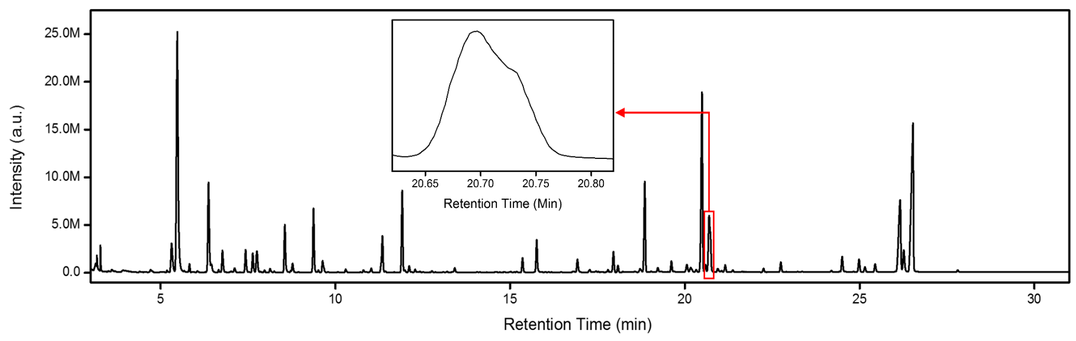


Figure 1: TIC of Rhizoma Chuanxiong with inset indicating the region of coeluted peak used for comparative study.

Analysis with SmartDalton™

ChemoPower's SmartDalton™ deconvoluted the co-eluted peak to reveal the presence of five unique components, C1–C5. Components C4 and C5 were designated as background noise while components C1, C2 and C3 were annotated as chemical compounds. The analysis is accurate since the surface plot of the GC-MS raw data revealed the presence of three unique components (Figure 2).

Analysis with Masshunter

Masshunter deconvolution algorithm is built upon the algorithm of AMDIS. This means that several parameter settings have to be inputted prior to analysis. Similarly to the analysis with AMDIS, the default settings were applied. Masshunter detected nine unique components, M1–M9.

Analysis with AMDIS

AMDIS applies an empirical-based algorithm that requires users to input parameter settings in order to perform peak deconvolution. In this study, the default settings were applied for analysis. Analysis with AMDIS revealed the presence of five unique components, A1–A5, as well. On closer observation, only components A1 has a proper peak profile. A2, A3 and A4 did not resemble a typical chromatographic elution profile and such inaccuracy prevents its usage for further quantitative analysis. Lastly, component A5 has a flat estimated TIC profile. The mass spectra of component A3 and A4 were clearly incomplete when compared to the mass spectrum of component C3 obtained by SmartDalton™ (Figure 3).

Conclusion

The comparison between three deconvolution algorithm, namely ChemoPower's SmartDalton™, AMDIS, and Agilent Masshunter, has shown that ChemoPower's deconvolution algorithm is capable of providing accurate identification of chemical compounds without the need for user-dependent inputs. More importantly, the extracted mass spectra are pure and clean, which will enable high confidence identification of chemical compounds

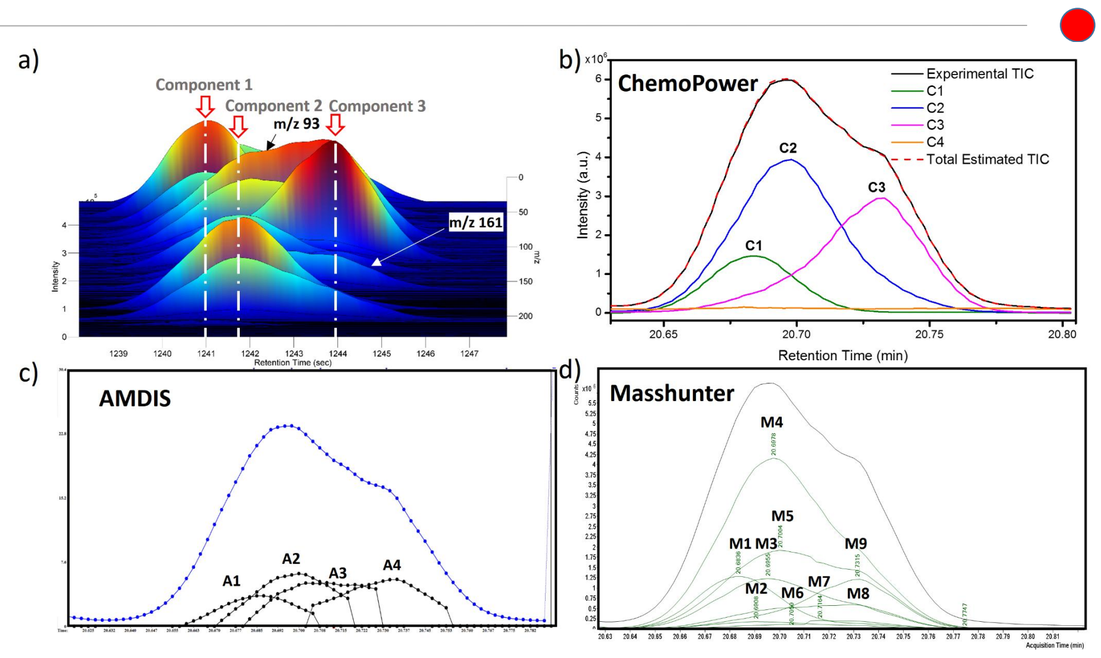


Figure 2. (a) Surface plots of raw GC-MS data. Deconvolution result of (a) ChemoPower, (b) AMDIS and (C) Masshunter.

Table 1: Analysis results upon library matching.

Components	Retention Time (min)	Chemical Name	Match Score	Retention index[a]	Chemical Formula
ChemoPower					
C1	20.6825	Pentadecane	913	1500	$C_{15}H_{32}$
C2	20.6975	α-Selinene	848	1494	$C_{15}H_{24}$
C3	20.7325	Bicyclogermacrene	840	1499	$C_{15}H_{24}$
AMDIS					
A1	20.6800	Pentadecane	909	1500	$C_{15}H_{32}$
A2	20.6980	α-Selinene	911	1494	$C_{15}H_{24}$
A3	20.7080	γ-Elemene	831	1434	$C_{15}H_{25}$
A4	20.7310	γ-Elemene	838	1434	$C_{15}H_{26}$
Masshunter					
M1	20.6836	Pentadecane	-	1500	$C_{15}H_{32}$
M2	20.6908	3-Hexenoic acid, 3-methyl-, methyl ester	-	(969)	$C_8H_{14}O_2$
M3	20.6955	(1S,2Z,5Z,9R)-2,6,10,10-Tetramethylbicyclo[7.2.0]undecan-2,5-diene	-	(1499)	$C_{15}H_{24}$
M4	20.6978	α-Selinene	-	1494	$C_{15}H_{24}$
M5	20.7004	2-hexyl-3-phenyl-oxirane	-	(1542)	$C_{14}H_{20}O$
M6	20.7050	1,4-Phthalazinediamine	-	(1842)	$C_8H_8N_4$
M7	20.7164	Trans-2-(3-Hydroxypropyl)cyclohexyl acetate	-	(1550)	$C_{11}H_{20}O_3$
M8	20.7288	4-(Ethoxycarbonyl)-1-(N-phenylureido)-3-[3-(17-oxoandrosta-3,5-dien-3-yl)propargyl]-2,5-dimethylpyrrole	-	(4914)	$C_{38}H_{45}N_3O_4$
M9	20.7315	rac-r-3-Acetoxy-1-(4-methoxybenzyl)-C-5-(2-thiazolyl)-2-pyrrolidinone	-	(2784)	$C_{17}H_{18}N_2O_4S$

* Retention index is based on semi standard non-polar values obtained from NIST library. Bracketed values are estimated values

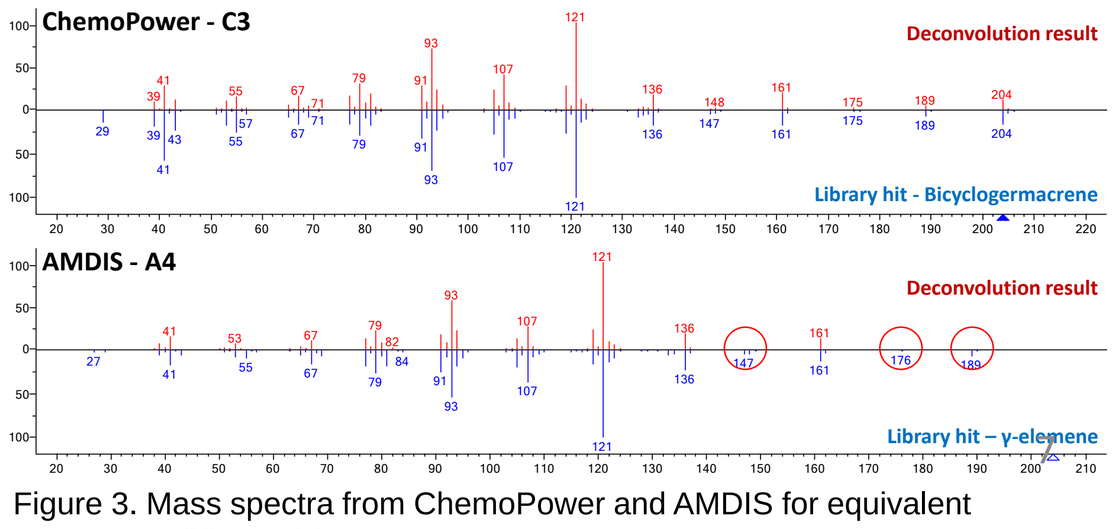


Figure 3. Mass spectra from ChemoPower and AMDIS for equivalent component C3 and A4.

Empower Your Research

References

- **Elimination of Matrix Interferences in GC-MS Analysis of Pesticides by Entropy Minimization**. B. Lu, Y. Lv, C. K. Chua, H. J. Zhang. J. Chin. Chem. Soc. 2017, 64, 804.
- **Dynamic background noise removal from overlapping GC-MS peaks via an entropy minimization algorithm.** C. K. Chua, Y. Lv, H. J. Zhang, X. Y. Gu. Anal. Methods 2017, 9, 2667

SmartDalton™

ChemoPower's patented technology - SmartDalton™ is a desktop client software that incorporates ChemoPower's proprietary peak deconvolution technique in GC-MS and LC-MS data analysis.

MoleculeDB™

ChemoPower's innovative software which enhances and simplifies NIST library matching in GC-MS and LC-MS data analysis. By using MoleculeDB™, users are able to identify chemical compounds and construct Proprietary Molecular Database in a very short time. It is on a cloud based server platform and it conducts chemical compound matching, head to tail analysis and scores matching.

ChemoPower's Homepage

OCAS: Online Chemical Analysis System

Our Partners

SHIMADZU Excellence in Science

ZBT 步長制藥 BUCHANG PHARMA

SPRING singapore Enabling Enterprise

A*STAR Institute of Materials Research and Engineering

A*STAR Institute of High Performance Computing

Ocean HEALTH Quality You Can Trust

asia natural products

HALTIA SERUM

ChemoPower Technology Pte Ltd
20 Science Park Road, #02-25 TeleTech Park
Singapore Science Park II, Singapore 117674
Tel.: (65) 6493 2780 Homepage: http://sg.ChemoPower.com
Email : contact@chemopower.com

www.chemopower.com

The Power of Chemometrics!

ChemoPower Singapore