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응용 자료

Automated Qualitative Analysis of Complex Mixtures Using ChromaLynx XS Software

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This is an Application Brief and does not contain a detailed Experimental section.

Abstract

This application brief highlights the capabilities of automated peak identification, library searching, and chromatogram comparison software within complex mixture analysis.

Benefits

Rapid detection, identification, and semi-quantitative determination of all components in complex mixtures

Introduction

Complex mixture analysis is a term that is applicable to a wide-range of MS application areas. A prerequisite is efficient chromatographic separation, whether performed by GC or ACQUITY UPLC. Typically data is acquired in full scan mode on a quadrupole or time-of-flight (ToF) mass spectrometer, such as the Waters GCT Premier or LCT Premier XE. ToF offers significant benefits such as improved full scan sensitivity, reduced cycle time, and high resolution.

The primary challenges for an analyst when reviewing acquired data are:

- · Identifying eluting peaks, primarily using library searching
- · Deconvoluting compounds where chromatographic separation is not complete
- · Comparing chromatograms to identify similarities or differences between acquired mixture samples

Each of these processes is time-consuming when performed manually, often resulting in a large number of printed chromatograms, mass spectra, library search results, and compound lists. A single data file could take hours to process, having only taken a few minutes to acquire, with a high probability for error during the manual process.

This technical note shows examples of the use of ChromaLynx XS Software for complex mixture analyses including:

- · Routine automated identification of peaks in complex chromatograms using deconvolution
- · Comparison of acquired data files such as comparing a known sample with a 'complaint' or tainted sample to

identify unique or common components

ChromaLynx XS offers a number of automated features to reduce the amount of time taken for these processes, and minimizes the possibility for errors compared with manual processing. Primary features include:

- · Automated high resolution deconvolution generating library searchable, background subtracted mass spectra
- · Automated exact mass scoring of library results
- · All results data stored in one interactive browser file
- · Chromatogram comparison highlights unique or common components between different acquired files

Experimental

Data acquisition and processing

Some representative data from the GCT Premier and LCT Premier XE were used, along with data acquired in EI+ and ESI+/- ionization modes.

All data were acquired using Waters MassLynxTM Software v. 4.1, with data processed using the ChromaLynx XS Application Manager.

Within ChromaLynx XS, acquired raw data files are processed from the sample list user interface, generating a single browser file that contains all of the information about the deconvoluted results:

- · Background subtracted mass spectra
- · Extracted exact mass chromatograms (XIC)
- · Library search results
- · Exact mass confirmation of library results

Results and Discussion

Figure 1 presents typical complex GC-MS and LC-MS chromatograms, which can be seen to contain a large

number of eluting peaks. To manually process these samples, identifying all 100 plus major peaks would take a considerable amount of time.

This process would require the generation of clean background subtracted spectra, sending the spectrum to a library search engine, and then collating the resultant library results. This does not include the added difficulties associated with deconvoluting close or partially co-eluting peaks or having to return to a previously searched peak. Automation of this process can save both time and reduce errors.

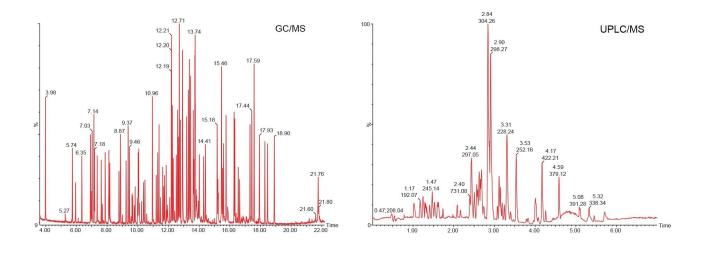


Figure 1. Typical complex GC-MS and UPLC-MS chromatograms.

Figure 2 shows the ChromaLynx XS browser window with identified peaks denoted using colored pointers. For the complex GC-MS chromatogram shown in Figure 1, ChromaLynx XS has automatically located, library searched, and exact mass scored a few hundred peaks in a matter of minutes.

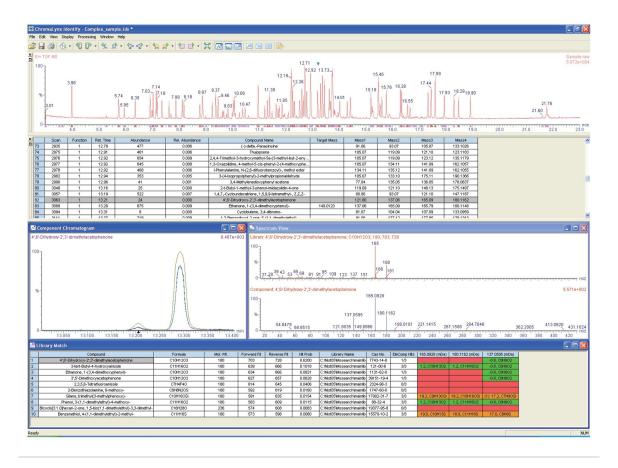
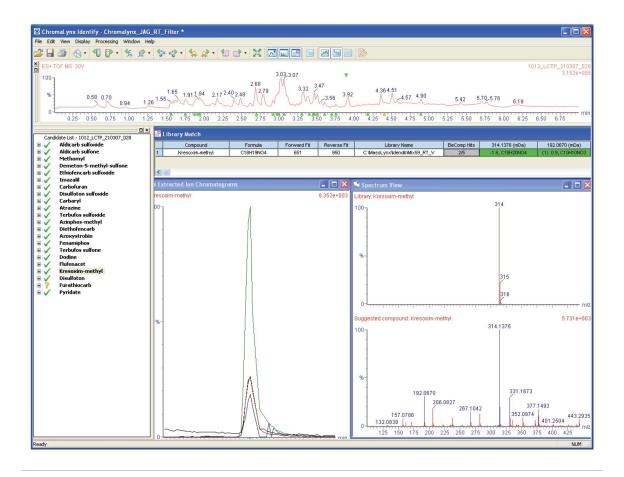
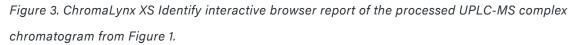


Figure 2. ChromaLynx XS Identify interactive browser report of the processed GC-MS complex chromatogram from Figure 1.

Figure 3 shows the ChromaLynx browser window for the complex UPLC-MS chromatogram, using an alternative candidate screening display, where only the compounds within a library are identified and highlighted.





Automated library fit assignment

Automated library fit results can be scored according to the exact masses acquired using high resolution ToF instruments. The correct library fit is difficult to assign using nominal mass information only. As shown in figure 4 (highlighted in green), nine out of the ten library fits have a molecular mass of 180, which correspond to the molecular ion in the acquired mass spectrum.

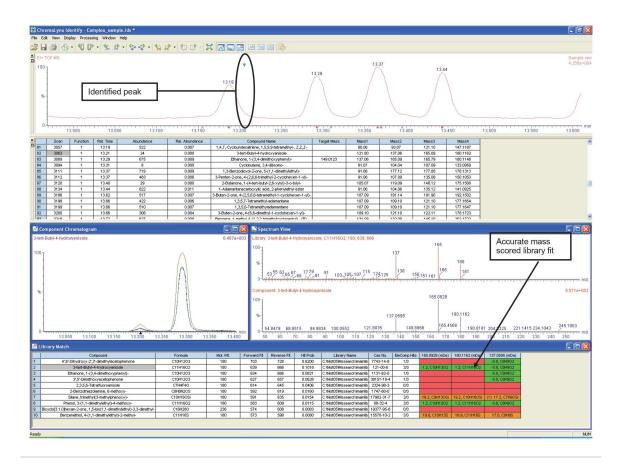


Figure 4. ChromaLynx XS Identify interactive browser highlights the capability of deconvolution and exact mass library scoring.

When comparing the acquired mass spectrum with the library spectra, it is difficult to assign a library fit with a high degree of certainty. This case highlights a situation where the high fullspectrum sensitivity of ToF has allowed a very low intensity peak to be detected. Because of the low intensity, it is very difficult to obtain good library fit results.

If the data had been acquired with nominal mass information only, selection of a tentative library fit would not be easy. By applying the exact mass capability, it is possible to propose that the most likely library hits are the result of compounds having the elemental composition $C_{11}H_{16}O_2$ which can now be easily distinguished from the compounds proposed by library search alone.

Exact mass scoring

Accurate mass scoring eases this process by automatically submitting each library entry's molecular composition to elemental composition calculation software. Within the processing setup, two thresholds can be specified:

1. The first threshold determines the mass accuracy that would give tentative agreement between the acquired and theoretical masses (low mass error).

2. A second threshold that specifies the mass deviation above which an acquired mass is high.

The deconvoluted masses for the acquired spectrum are then displayed, highlighted using colored backgrounds. Green shows a deviation of between zero and the tentative (low) threshold; amber shows a deviation between the low and high thresholds; and red shows where the mass deviation is above the high threshold. In this case, the second and eighth library fits are supported by the exact mass scoring of the molecular and fragment ions, as shown in Figure 4. Manually generating this information would be laborious, with a high probability of error.

Manual comparison

Manual comparison of chromatograms is another time-consuming process that can be automated by using ChromaLynx XS. When using the Compare feature, reports can be generated that specify what the common or unique components in complex mixtures are. This is a common process when investigating complaints within the flavor and fragrance, food, fine chemicals, or environmental industries.

Often the differences between chromatograms can highlight issues resulting from adulteration, tainting, or contamination of products or sample matrices (essential oils, soil, drinking water, etc.).

The browser window shown in Figure 5 compares a premix essential oil with a peppermint essential oil. Although ChromaLynx XS does not perform detailed quantification, it can compare peak areas, either against each other or against the total ion count (TIC). Here, the two complex mixtures have been compared on a mass and retention time basis, with QC scoring highlighting a pair of common peaks that also have similar area counts (in this case, a difference of less than 20% between the two samples).

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GCTP_281108_014 28 1562 9.2401 1605 0.023 Cyclohexanone, 5-methyl-2(1-methylethyl), (25-4r 1 0.0018 1 0.9490 20 ✓		GCTP_291106_014 51 2655 12.8846 1386 0.020 Longitalene-(V4) 0 0.0002 0 0.2500 20 X	Sample Name D Scan GCTP_291106_014 4 467 GCTP_291106_014 5 651 GCTP_291106_014 6 882 GCTP_291106_014 9 89 GCTP_291106_014 10 919 GCTP_291106_014 10 919 GCTP_291106_014 20 1519	5.5906 6.2030 6.3069 7.0208 7.0972 9.0971	stative Retention Time	385 211 701 84 831 5682	0.006 0.003 0.010 0.001 0.012 0.083	3-Carene 1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)- Cyclohexaene, 4-methyleme-1-(1-methylethyl)- 1,3,8-p-Merthatriene Cyclohexaene, 1-methyl-5-(1-methyletheryl)-, (R)- Cyclohexaene, 5-methyl-2-(1-methylethyl)-	0 0 1 0 0 1	0.0031 0.0030 0.0027 0.0027 0.0020 0.0020	1 1 1 1 1 0	0.1878 0.0736 0.4693 0.3621 0.2715 49.8677	20 20 20 20 20 20 20	×××××		į.
			Sample Name D Scan OCTP_201106_014 4 467 OCTP_2201106_014 5 651 OCTP_2201106_014 9 868 OCTP_2201106_014 9 968 OCTP_2201106_014 10 919 OCTP_2201106_014 20 1502 OCTP_201106_014 20 1502	5.5906 6.2030 6.3069 7.0208 7.0972 9.0971 9.0971 9.2401	stative Retention Time	385 211 701 84 831 5682 1605	0.006 0.003 0.010 0.001 0.012 0.083 0.023	3-Carene 1,4-Cyclohexadere, 1-nethyl-4(1-methylethyl)- Cyclohexane, 4-nethyl-6-1(1-methylethyl)- 1,3,8-p.Merthatriene Cyclohexanone, 5-methyl-2(1-methylethyl)- Cyclohexanone, 5-methyl-2(1-methylethyl)- (2)-Strip-2-2-1-methylethyl)- Cyclohexanone, 5-methyl-2(1-methylethyl)- (2)-Strip-2-2-1-methylethyl)- (2)-Strip-2-2-1-methylethyl)- (2)-Strip-2-2-1-methylethyl)- (2)-Strip-2-2-1-methylethyl)- (2)-Strip-2-2-1-methylethyl)- (2)-Strip-2-2-1-methylethyl)- (2)-Strip-2-2-2-2-2-2-2-2-2-2-2-2-2-2-2-2-2-2-2	0 0 1 0 0 1 1	0.0031 0.0030 0.0027 0.0027 0.0020 0.0004 0.0018	1 1 1 1 1 0 1	0.1878 0.0736 0.4693 0.3621 0.2715 49.8677 0.9490	20 20 20 20 20 20 20 20 20	×××××		
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5 COT2, 281106, 014 10 919 7.0972 031 0.012 Crychetherens, 1-methys-61-(-methyserper), (Pt) 0 0.0020 1 0.27715 20 6 COT2, 281106, 014 20 30571 5822 0.003 Crychetherens, 1-methys-61-(-methyserper), 10004 0 48.877 20 7 SORTE, 281106, 014 2 1952 2.4201 10056 0.023 Crychetherens, 5-methy-62-(-methyserper), 52-methy 1 0.0014 0 48.877 20 V 7 SORTE, 281106, 014 2 1952 2.4201 10056 0.023 Crychethystres, 5-methy-62-(-methystres, 5-methys-62-(-methystres, 5-methys-62-(-methystres, 5-methys-62-(-methystres, 5-methystres, 5-			GCTP_291106_014													
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oc179_391108_014 53 2888 13.8807 1510 0.022 Cyclohexone, 6-ethery/6-4-nethyl-1-(1-exethylethyl) 1 0.0021 1 2.8728 20 🗙			Sample Name D Scan QCTP_231106_014 4 467 QCTP_231106_014 5 561 QCTP_231106_014 6 562 QCTP_231106_014 6 862 QCTP_231106_014 10 919 QCTP_231106_014 10 919 QCTP_231106_014 20 562 QCTP_231106_014 20 2000 QCTP_231106_014 50 2050 QCTP_231106_014 51 2050 QCTP_231106_014 51 2050	5.5906 6.2030 6.3069 7.0208 7.0972 9.0971 9.9.2401 1.2.3942 5.12.8846	Solve Retension Time	385 211 701 84 831 5682 1605 231 1386	0.006 0.003 0.010 0.012 0.083 0.023 0.003 0.020	3-Cerene 1.4-Cyclohrowdre, 1.eethyl-44(-eethylethyl)- Cyclohezone, 4-anthylethyl-1(1-anthylethyl)- 1.3.8-p-Martinatrane Cyclohezonen, 5-anthyl-2(1-anthylethyl), (B)- Cyclohezonen, 5-anthyl-2(1-anthylethyl), (C3-4- Cyclohezonen, 5-anthyl-2(1-anthylethyl-2(1-anthylethyl), (C3-4- Cyclohezonen, 5-anthyl-2(1-anthylethyl), (C3-4- Cyclohezonen, 5-anthyl-2(1-anthylethyl), (C3-4- Cyclohezonen, 5-anthyl-2(1-anthylethyl), (C3-4- Cyclohezonen, 5-anthyl-2(1-anthylethyl), (C3-4- Cyclohezonen, 5-anthyl-2(1-anthylethyl), (C3-4- Cyclohezonen, 5-anthyl-2(1-anthylethyl)), (C3-4- Cyclohezonen, 5-anthyl-2(1-anthylethyl))), (C3-4- Cyclohezonen, 5-anthylethyl)), (C3	0 0 1 0 1 1 1 0 0	0.0031 0.0030 0.0027 0.0027 0.0020 0.0004 0.0018 0.0002 0.0002	1 1 1 1 0 1 0 0 0	0.1878 0.0736 0.4683 0.3621 0.2715 49.8677 0.9490 0.7112 0.2500	20 20 20 20 20 20 20 20 20 20 20 20	×××××	[
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Figure 5. ChromaLynx XS Compare interactive browser showing the common components between premix and peppermint essential oils.

This QC scoring is highlighted by assigning a green tick to the peak in question. The Compare report shows that there are not many common peaks, indicating that ten compounds are common with one compound present at a similar intensity when comparing the premix and peppermint essential oils.

ChromaLynx XS Compare can also display the unique components detected within different samples, as shown in Figure 6. In this case, peppermint oil is not one of the constituent components of the premix oil, so a much larger number of unique components are being highlighted.

Chromal.ynx Compare - 1011_Es Edit View Display Processing Wi		s *												
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GCTP 291106 015														
	Detection Time	Relative Retention Time	6 human langes	Detettus Aburatana	Compound Name	Columbust Dealer	Date DT	Date Care	Abundance Ratio	OC LINE (W)	OC Data			٦
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GCTP_291106_015 9 713 GCTP_291106_015 10 809			213	0.003	Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)- è-Phellandrene	0	-							
GCTP 291106 015 13 822			2082	0.032	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	1								
GCTP_291106_015 17 930			626	0.010	3-Carene	1								
GCTP_291106_015 18 123	8.1514		761	0.012	Bicyclo[4.1.0]hept-3-ene, 3,7,7-trimethyl-, (1S)-	0								
GCTP_291106_015 19 129			312	0.005	2H-Pyran, tetrahydro-4-methyl-2-(2-methyl-1-prope	0								
GCTP_291106_015 20 1370			171	0.003	9-Ethylbicyclo(3.3.1)nonan-9-ol	0	-							
GCTP_291106_015 22 152 GCTP_291106_015 26 180			294 3567	0.004	Acetic acid, phenylmethyl ester Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1å,36,6	0	-							
GCTP_291106_015 26 180.			1219	0.019	3-Carene	1					+			
OCTP_291106_015 28 2005			1830	0.028	Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	1								
GCTP_291106_015 30 211:	11.0734		367	0.006	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	0								
GCTP_291106_015 31 2290			653	0.010	Cyclohexene, 4-ethenyl-4-methyl-3-(1-methylethen	0								
GCTP_291106_015 32 2343 GCTP_291106_015 33 2469			59 1336	0.001	2,4-Quinolinediol	0	_							
GCTP_291106_015 33 246	12.2664		1336	0.020	Copaene	1			l					
GCTP_291106_014														
Sample Name ID Scan	Retention Time	Relative Retention Time	Abundance	Relative Abundance	Compound Name	Saturated Peaks	Delta RT	Delta Scan	Abundance Ratio	QC Limit (%)	QC Pass			
GCTP_291106_014 2 9	4.0644		191	0.003	Perfluoro(2-methylpentane)	0								
GCTP_291106_014 3 14	4.0796		321	0.005	Perfluorotributylamine	0								
GCTP_291106_014 7 713 GCTP_291106_014 8 860	6.4120		48	0.001	Cyclopentadiene, 2,5,5-trimethyl- (+)-4-Carene	0	-							
GCTP_291106_014 8 880 GCTP_291106_014 12 939	7.1642		3352	0.049	Eucalyptol	1								
GCTP_291106_014 12 838 GCTP_291106_014 13 1053	7.5455		280	0.004	1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-	0								
GCTP_291106_014 15 1114	7.7484		672	0.010	1,4-Cyclohexadiene, 1-methyl-4-(1-methylethyl)-	0								
GCTP_291106_014 16 1511	9.0718		6	0.000	3-Buten-2-one, 4-(diethylamino)-4-(dimethylamino)-	0								
GCTP_291106_014 17 1512	9.0750		121	0.002	2,5-Pyrrolidinedione, 3-(1-chloroethyl)-4-methyl-	0								
GCTP_291106_014 21 1521 GCTP_291106_014 22 1525	9.1036		558 20	0.008	6-Methyl-cyclodec-5-enol 1H-Azepine, 2,3,4,5,6,7-hexahydro-2-octylinino-	0	-							
GCTP_291106_014 22 1525 GCTP_291106_014 23 1537	9.1195		20	0.000	TH-Azepine, 2,3,4,5,6,7-hexanydro-2-octylimino- Cyclohexane, 1-methyl-3-propyl-	0	-	-			<u> </u>			
GCTP_291106_014 24 1550	9.2029		1605	0.023	2-Cyclopenten-1-one, 2-(2-butenyl)-3-methyl-, (Z)-	1		-						
GCTP_291106_014 26 1552	9.2068		2280	0.033	2-Cyclopenten-1-one, 2-(2-butenyl)-3-methyl-, (Z)-	1								
GCTP_291106_014 29 1578	9.2949		1403	0.020	Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1à,3á,6	1								
GCTP_291106_014 30 1579	9.2973		967	0.014	Cyclohexene, 1,4,6,6-tetramethyl-	1								
	9.3692		14	0.000	Phenol, 2-cyclohexyl-4-methyl-	0	1	1	1	1	1			
GCTP_291106_014 31 1600 GCTP_291106_014 32 1604	9.3811		5	0.000	4-Hydroxy-2-hydroxymethyl-6-methylpyrimidine	0								

Figure 6. ChromaLynx XS Compare interactive browser showing the unique components within each sample of premix and peppermint essential oils.

Conclusion

- ChromaLynx XS streamlines the workflow within the investigative laboratory by reducing the time spent on the laborious manual tasks of locating and identifying chromatographic peaks.
- There is a reduced risk of errors, since all of the information is stored within a single results browser file eliminating the need for endless printouts of background subtracted mass spectra and library search results from different programs.
- The ability to automatically compare samples saves time and reduces errors by providing comparative information in an easy-to-view and rapid manner.

· ChromaLynx XS Software offers:

- The rapid detection, identification, and semi-quantitative determination of all components in complex mixtures.

- The combination of non-targeted component detection with a library search to facilitate identification.

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720002643, July 2008

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