APPLICATION NOTE

Fragrance Screening and Profiling using GC-MS equipped with FFNSC Library

AN187v1; SCION Instruments

Introduction

Fragrances are complex mixtures which can be made up of both natural and synthetic aromatic compounds. The International Fragrance Association (IFRA) defines a fragrance as "a mixture of ingredients designed to produce a pleasant or distinctive smell".[1] These mixtures can be formed of numerous subtly different compounds, which are often almost identical but work together to produce these desired distinctive smells.

GC-MS can help to unlock these complex mixtures by identifying key components of a fragrance giving a greater understanding of a product and allowing for easy reproduction in the manufacturing process.

"A single scent can unlock memories, change your mood, or make a moment unforgettable".[1]

The SCION 8700 MS combined with the FFNSC (Flavors and Fragrances of Natural and Synthetic Compounds) spectral library facilitates identification of unknown compounds in complex mixtures allowing for the detection of undesired impurities and for flavour profiling. The spectral library, FFNSC 3, contains 3462 mass spectra specific to compounds in the flavours and fragrance industry.

Flavour profiling allows the user to define a products' unique sensory fingerprint. This can be a powerful tool when developing new products or trying to reverse engineer an existing product.

For quantitative targeted analysis of the IFRA 57 allergens see our Application Note on the SCION Instruments website.

In this application note we will look at a number of different functions and highlights of the SCION 8700 MS and MSWS software which allow for easy screening and profiling of fragrance products with the use of the FFNSC 3 spectral library.

Experimental

4 fragrance products (named Sample 14, 15, 16, and 17) provided by a SCION Instruments customer were used to demonstrate the ability of the SCION 8700 GC-MS and FFNSC 3 library for screening and profiling.

A generic screening method was employed, instrument parameters can be found in Table 1.

Depending on the nature of the samples being analyzed often injections can be made with the neat product, sometimes a simple dilution in solvent might be employed or in more complex cases (formulations, etc) an extraction may be performed to remove interfering matrix effects.

Table 1 Instrument Conditions

GC Part	Settings
Injector	200°C Split 20:1
Injection Volume	1.0 µL
Column	SCION-5MS 30m x 0.25mm x 0.25µm
Carrier Gas	Helium 1.5 mL/min
Oven Program	50 °C (hold 2.0 min), 5 °C/min to 250 °C (hold 8.0 min)
Run Time	50 min
Software	MSWS with FFNSC 3 Spectral Library
MS Part	**Settings**
MS transfer line temp	250 °C
Ion source temp	250 °C
MS mode	Electron Ionization
Delay collection time	3.50 min
Scan mode	Full Scan (50 – 500 amu)

In this instance the products were diluted in isooctane by weighing 50 mg of each product into separate 5 mL volumetrics, these were then made to volume with isooctane to give 10 mg/mL solutions. The samples were then injected onto the GC-MS. Isooctane blanks were ran to prevent false identification of compounds.

Results

In the following sections we will look at several different functionalities within MSWS which combined with the FFNSC library allows for easy screening and profiling of fragrance products.

The topics covered here are supported by our software guides which contain step by step instructions on how to perform the actions described in this application note. Videos can be found on the SCION Instruments YouTube channel.

Fragrance Screening and Profiling using GC-MS equipped with FFNSC Library

AN187v1; SCION Instruments

Manual Peak Searching

The first function in MSWS we will cover is manual peak searching, this is where the user defines which specific peak they wish to perform a library search on to determine the likely identity of that peak. Typically this is done when a user already has an idea of the make up of a particular sample and wants to focus on a specific region within the resulting total ion chromatogram (TIC).

Figure 1 shows the TIC of a fragrance product "Sample 14".

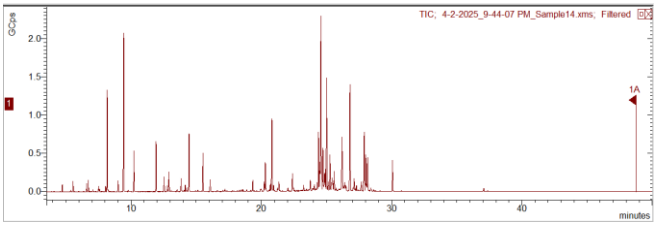


Figure 1 TIC of Sample 14

The user is able to simply zoom in on a specific target area and perform individual library searches on desired peaks. Figure 2 shows an example expanded chromatogram of sample 14 with the resulting mass spectra from the selected peak at 20.81 minutes.

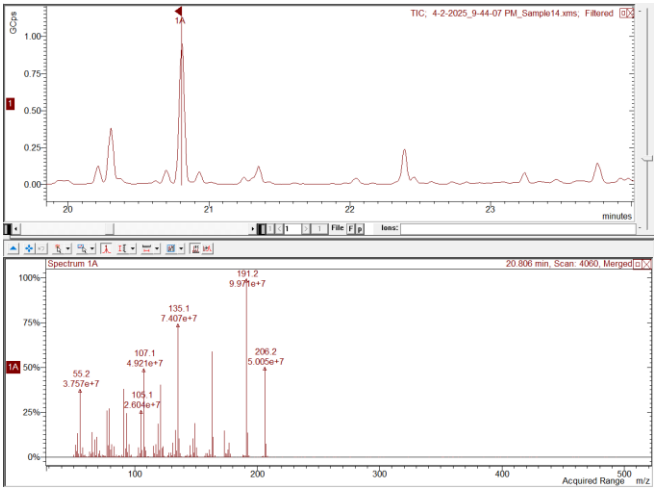


Figure 2 Enhanced TIC of Sample 14 (Top) with resulting mass spectra from selected peak @20.81 min

The user can then perform a library search using the integrated search function tool and FFNSC library within MSWS. Figure 3 shows the library match report generated from the selected mass spectra. If multiple matches appear the user can easily navigate between them and choose the most likely match. See our technical note on "NIST library compound scoring GC-MS" for more information on how to do this in the SCION Instruments knowledge centre.

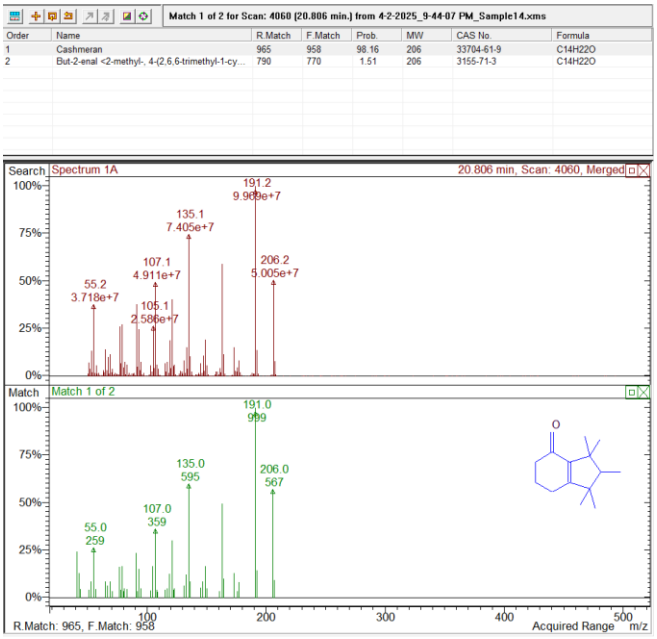


Figure 3 Library search results for unknown peak @20.81 min

In Figure 3, the top match is Cashmeran which is clearly the most likely the identity of the unknown compound (red) due to the mass spectrum match (green). There are a number of qualitative reporting options available with guides on how to use these on the SCION Instruments YouTube channel.

Automatic Peak Searching

The second function we will cover is automatic peak searching, this is where the user utilizes the "integrate" function within the TIC window. This allows integration of multiple peaks based on the conditions the user has input (peak width, sensitivity, minimum peak size, etc). Typically this is used with unknown samples where a user wants to build a picture about the nature of the compounds present. This is also known as profiling. Figure 4 shows example integration parameters used with Figure 5 showing the integrated TIC. Figure 6 shows an expanded TIC.

Once integrated the software generates a simple % area report which can be exported/printed and gives a good basic overview of the presence of each compound.

An additional powerful tool available to the user is the ability to export the mass spectra of all integrated peaks to a spectrum list. This spectrum list can then be used to do a library search for all compounds instantly. Within this function there is the ability to tailor the search parameters which can be very useful for an advanced user.

Fragrance Screening and Profiling using GC-MS equipped with FFNSC Library

AN187v1; SCION Instruments

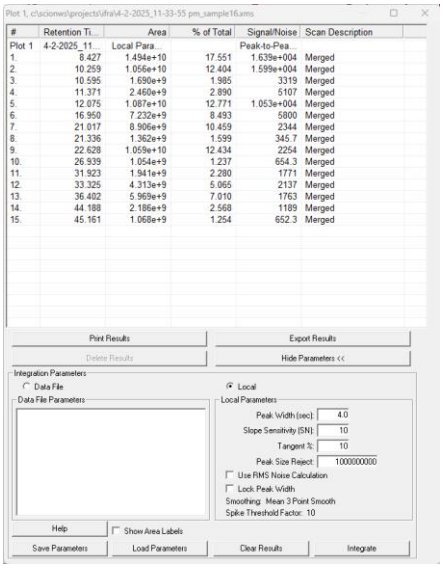


Figure 4 Example integration parameters and generated report of integrated peaks from Sample 16

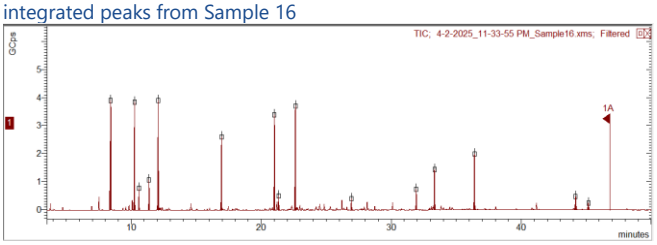


Figure 5 Integrated TIC of Sample 16 showing integrated peaks

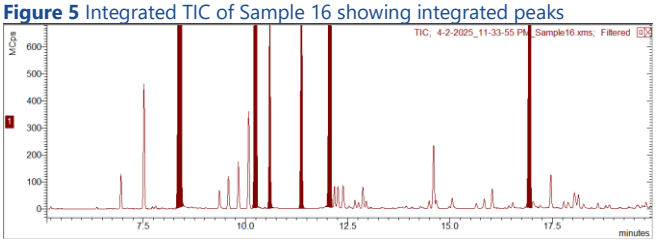


Figure 6 Expanded TIC showing integrated peaks of Sample 16

Figure 7 shows the search parameters available when library searching a spectrum list. The user has the ability to chose which libraries are active (including custom user libraries) as well as more advanced options such as limiting the mass range, number of hits, and threshold of matches.

Figure 8 shows the library match compounds generated for the 15 integrated peaks taken from Sample 16. The user has the ability to quickly review each match and if desired can investigate other matches if they believe the library has an incorrect match.

The user can generate qualitative reports with these results or can export the spectrum list with an updated compound table (named peaks) to either the original full scan method for enhanced qualitative or semi quantitative analysis, or create a new SIM method for targeted quantitative analysis.

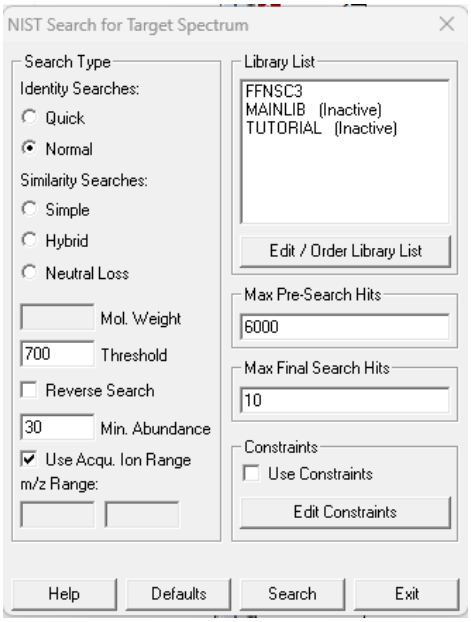
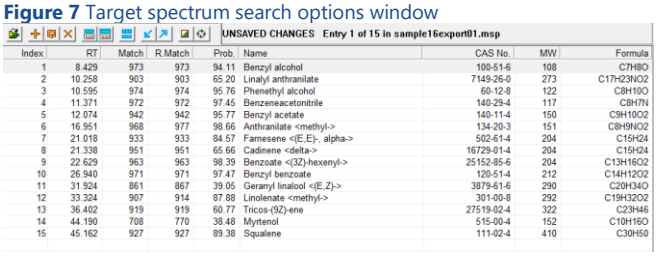


Figure 7 Target spectrum search options window



UNSAVED CHANGES Entry 1 of 15 in sample16export01.msp

Index	RT	Match	R.Match	Prob.	Name	CAS No.	MW	Formula
1	8.429	973	973	94.11	Benzyl alcohol	100-51-6	108	C7H8O
2	10.258	903	903	65.20	Linalyl anthranilate	7149-26-0	273	C17H23NO2
3	10.595	974	974	95.76	Phenethyl alcohol	60-12-8	122	C8H10O
4	11.371	972	972	97.45	Benzeneacetonitrile	140-29-4	117	C8H7N
5	12.074	942	942	95.77	Benzyl acetate	140-11-4	150	C9H10O2
6	16.951	968	977	98.66	Anthranilate <methyl->	134-20-3	151	C8H9NO2
7	21.018	933	933	84.57	Farnesene <(E,E)-, alpha->	502-61-4	204	C15H24
8	21.338	951	951	65.66	Cadinene <delta->	16729-01-4	204	C15H24
9	22.629	963	963	98.39	Benzoate <(3Z)-hexenyl->	25152-85-6	204	C13H16O2
10	26.940	971	971	97.47	Benzyl benzoate	120-51-4	212	C14H12O2
11	31.924	861	867	39.05	Geranyl linalool <(E,Z)->	3879-61-6	290	C20H34O
12	33.324	907	914	87.88	Linolenate <methyl->	301-00-8	292	C19H32O2
13	36.402	919	919	60.77	Tricos-(9Z)-ene	27519-02-4	322	C23H46
14	44.190	708	770	38.48	Myrtenol	515-00-4	152	C10H16O
15	45.162	927	927	89.38	Squalene	111-02-4	410	C30H50

Figure 8 Library matches for the spectrum list (15 compounds) exported from Sample 16

More information on quantitative analysis for fragrances compounds can be found in our application note IFRA 57 Allergens on the SCION Instruments website.

Target List Search

The final function we will demonstrate is the "Target List Search" tool. This allows a user to easily screen chromatograms for target compounds.

This is especially useful for fragrance compounds which can be incredibly complex and contain a vast numbers of often similar compounds.

The user can build a target list of desired compounds to screen either directly from the FFNSC, or any library including custom user libraries built from their own data.

The target list search function will then scan a chromatogram and generate a report on whether a match has been found for each compound. For the following examples, we have built a spectrum list using 5 entries from the FFNSC library; benzyl alcohol, methyl anthanilate, methyl hexadecanoate, hexenyl benzoate, and dihydromyrcenol.

Fragrance Screening and Profiling using GC-MS equipped with FFNSC Library

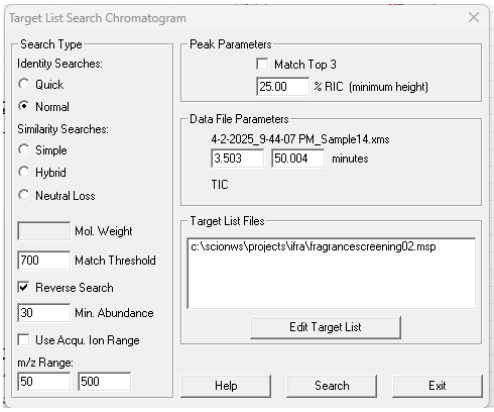


Figure 9 Target List Search Chromatogram Options

Figure 9 shows the search options available. The user is able to limit mass range, response, match threshold and other variables to enhance the search.

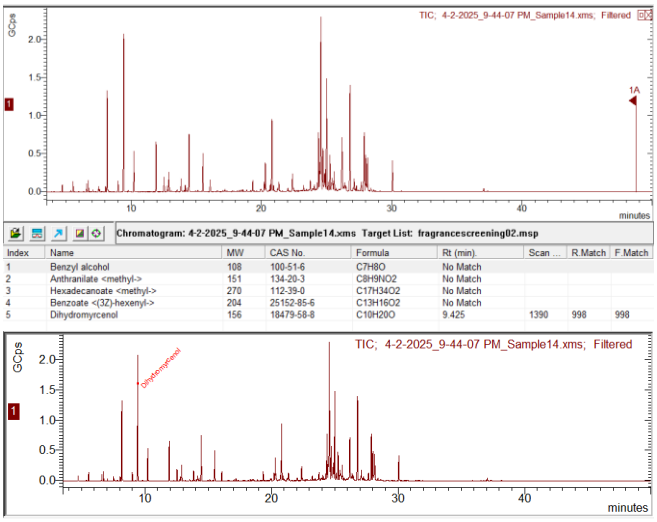


Figure 10 Showing Sample 14 unprocessed TIC (top), target list search result table (middle) and processed TIC with compound match (bottom)

With this spectrum list we are now able to perform a Target List Search. This quickly screens the entire chromatogram and produces a match list report as well as giving a visualisation through a processed TIC showing the position of any positive matches. This tool is an incredibly powerful and efficient screening technique allowing for even a novice user to effortlessly screen complex data for target compounds.

Once identified the user then has the option to produce qualitative reports or further process the data for semi quantitative analysis. SIM methods can also be easily built for true quantitative analysis for subsequent samples. Figures 10, 11, 12, and 13 show target list search results for samples 14, 15, 16 and 17 respectively.

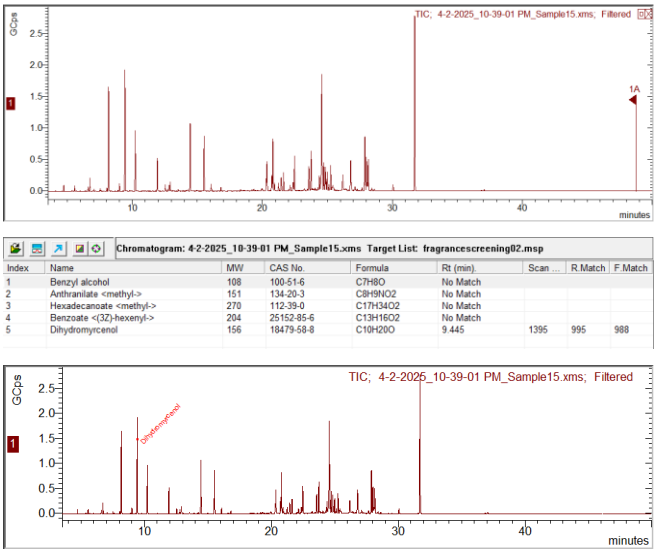


Figure 11 Showing Sample 15 unprocessed TIC (top), target list search result table (middle) and processed TIC with compound match (bottom)

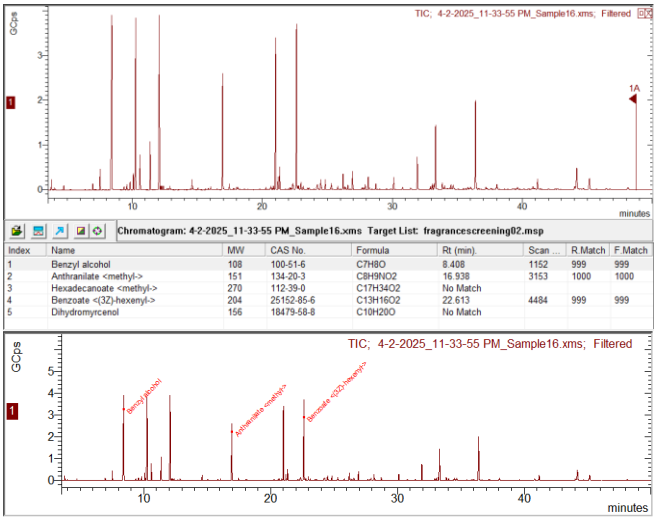


Figure 12 Showing Sample 16 unprocessed TIC (top), target list search result table (middle) and processed TIC with compound match (bottom)

Fragrance Screening and Profiling using GC-MS equipped with FFNSC Library

AN187v1; SCION Instruments

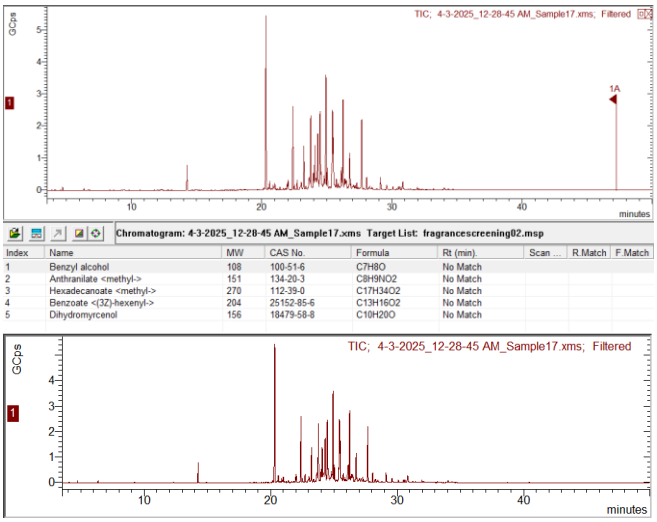


Figure 13 Showing Sample 17 unprocessed TIC (top), target list search result table (middle) and processed TIC with compound match (bottom)

The target list search results showed positive matches for dihydromyrcenol in samples 14 and 15. Sample 16 showed matches for benzyl alcohol, methyl anthanilate, and hexenyl benzoate with Sample 17 having no positive matches. This shows how effective a screening tool the target list search function is, even with very complex sample matrices.

Conclusion

In this application note we have explored a number of different functions and highlights of the SCION 8700 MS and MSWS software which allowed for easy screening and profiling of fragrance products with the use of the FFNSC 3 spectral library.

4 fragrances from a SCION Instruments customer were prepared by a simple dilution and then analyzed alongside solvent blanks to prevent false identifications. It was shown how to utilize the functionalities in MSWS, manual and automatic peak searching and target list searching, to screen samples for impurities and flavour profiles.

SCION Instruments recommends checking with local regulatory authorities to ensure all testing and reporting requirements are met, or contact the SCION applications team for assistance.

References

1. IFRA, https://ifrafragrance.org/about-fragrance/this-is-a-fragrance, (accesed Feb 2026)

Order Information

Ordering Information for the 8300 GC	
Part	**Part Number**
8300 GC with 8700-MS-SQ EI Select, with S/SL inlet (120V)	SCIONSQ83SEL311
8300 GC with 8700-MS-SQ EI Select, with S/SL inlet (230V)	SCIONSQ83SEL312
8400 PRO Autosampler for 8300 GC and 8500 GC	840000001
FFNSC 3.0 – Mass Spectral Database	394105201
Suggested Consumables	
Part	**Part Number**
15% Graphite/85% Vespel Ferrule 1/16" with 0.4 mm hole pk/10	41312148
BTO Septa 9 mm, pk/50	CR298713
10µL fixed needle syringe, 5 cm, 0.47 mm OD, 26 g conical needle	41312133
SCION-5MS column 30m x 0,25mm x 0,25 µm	SC32223
LINER 1177 78.5 L x 6.3 OD x 4MM ID S/SL FOCUS PK/5	41312101

SCION offers other MS options such as the 8700 SQ Premium and 8900 TQ, as well as additional spectral libraries such as Designer Drugs and Wiley, please contact your local SCION sales representative to discuss your needs.

For more information, please contact:

E: sales-eu@scioninstruments.com

W: www.scioninstruments.com