

msFineAnalysis iQ Ver.2 Target Analysis Example I Rapid Analysis of Food Aroma Components

Product used : Mass Spectrometer (MS)

1. Introduction

Target Analysis is a method for fast and accurate search and evaluation of only the target compounds based on integrated qualitative analysis¹⁾ with EI and Soft Ionization (SI) data. In this method, it is necessary to register the CAS RN®, molecular formula (or molecular weight), fragment composition formula of target compounds in the "Target List" in advance. Based on the registered information, each extracted ion chromatogram (EIC) is plotted for EI and SI measurement data and peaks are detected. The molecular ion peak in the mass spectrum, its isotopic pattern, similarity and retention index with the NIST database are confirmed on the detected peak. These results are used to determine whether or not it is the target compound. This time we report the results of the analysis of optional aromatic components from the volatile organic compounds of hamburger using this method.

2. Experiment

A commercial hamburger weighing 7.5 g was used as a sample. Volatile compounds were extracted using a microchamber (µ-CTE250, MARKES International Ltd.) and measured using a GC-MS (JMS-Q1600GC, JEOL Ltd.) equipped with a TD pre-treatment device (TD-Xr100, MARKES International Ltd.). The ionization methods used were EI and PI as SI. The data obtained were analyzed using the "Target Analysis" function in the integrated qualitative analysis software called msFineAnalysis iQ. The measurement conditions are shown in Table 1. (MSTips No.485)



TD-Xr100-JMS-Q1600GC UltraQuad[™] SQ-Zeta



Ion source (Share use of EI/PI)

Parameter		Value							
Micro- Chamber	Sampling	30 ℃(10 min), 50 mL/min (N2)							
	Sample tube type	Tenax TA							
TD	Tube desorption	250 °C(10 min), 50 mL/min, Splitless							
	Trap desorption	25-300 °C(3 min), 50 mL/min, Split (1/3.5)							
	Column	Inart Cap Pure-WAX (GL Science, inc.), 60 m ×0.25 mm id, 0.25 µm film							
GC	Column flow	2.0 mL/min (He)							
	Oven temp.	40 ℃(3 min)-8 ℃/min-250 ℃(5.75 min)							
	Inlet temp.	200 °C							
	Interface temp.	230 °C							
	Ion source temp.	200 °C							
MS	Ionization	EI (70 eV, 50 μΑ) PI (approx.10 eV, Fil.Off)							
	Scan rango	m/z 29-400							

Table 1 Measurement Condition

3. Results

3.1 TICC

The GC/EI TICC of thermal desorption is shown in Fig.1. Mainly, aroma components presumed to originate from hamburger such as acetic acid, Acetoin and 1-Butanol-3-methyl, etc. were confirmed. From the "Target Analysis", seven types of components originating from herbs and spices were estimated.



Fig.1 GC/EI TIC chromatogram

Table 2 Target list

	No.	Name	CAS#	NIST Library	EIC Creation	Molecular Formula	Fragment Formula	m/z (EIC)	RT [min]	RI [iu] Non-Polar	RI [iu] Semi Non-Polar	RI [iu] Polar	Description	Spectrum	
	001	1-Carvone	99-49-0	1	Molecular Io	C10H14O		150		1218	1242	1739	Caraway	View	^
	002	Eugenol	97-53-0	1	Molecular lo	C10H12O2		164		1335	1357	2169	Basil	View	
	003	α-Phellandrene	99-83-2	1	Molecular lo	C10H16		136		998	1005	1167	parsley	View	
	004	1-Butene, 4-isothiocyanato-	3386-97-8	1	Molecular Io	C5H7NS		113		964	983	1453	mustard	View	
	005	β-Pinene	127-91-3	1	Molecular lo	C10H16		136		973	979	1112	pepper	View	
	006	Diallyl disulphide	2179-57-9	1	Molecular Io	C6H10S2		146		1069	1081	1475	garlic	View	
	007	Vanillin	121-33-5	1	Molecular Io	C8H8O3		152		1361	1404	2568	vanilla	View	~

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3.2 Result of target analysis

The result of the target analysis is shown in Fig.2. The aroma components of the hamburger were estimated as caraway, basil, parsley and pepper in the target list. See the blue background color.

	Background color : white more peak detected, yellow more a detected, blue more beak detected and clear target judgment											
Target Information												
ID	List Name Name		CAS#	NIST Library	Molecular Formula	Fragment Formula	m/z (EIC)	RT [min]	RI [iu]	Description	Num. of Detected	Num. of Passed
T001	Targetlists_self	1-Carvone	99-49-0	 Image: A set of the set of the	C10H14O	-	150	-	1739	Caraway	7	1
T002	Targetlists_self	Eugenol	97-53-0	 Image: A set of the set of the	C10H12O2	-	164	-	2169	Basil	3	1
T003	Targetlists_self	α-Phellandrene	99-83-2	 Image: A set of the set of the	C10H16	-	136	-	1167	parsley	30	2
T004	Targetlists_self	1-Butene, 4-isothiocyanato-	3386-97-8	~	C5H7NS	-	113	-	1453	mustard	0	0
T005	Targetlists_self	β-Pinene	127-91-3	 Image: A second s	C10H16	-	136	-	1112	pepper	30	2
T006	Targetlists_self	Diallyl disulphide	2179-57-9	 Image: A second s	C6H10S2	-	146	-	1475	garlic	8	0
T007	Targetlists_self	Vanillin	121-33-5	 Image: A second s	C8H8O3	-	152	-	2568	vanilla	3	0

Fig.2 Target information

3.3 Details of target analysis results for [ID:T003]

As an example, details of the target analysis results for compound ID:T003 are described. The EIC (m/z 136) specified in T003 is plotted from the EI and PI measurement data. The peaks in the PI data plotted by EIC(m/z 136) are shown in Fig.3. Figure 4 shows the target judgment result for the RT10.04 minute peak in Figure 3. The result shows that the spectral similarity is 757 (Max:999), the measurement error of RI (Δ RI) is -13 [iu]. In addition, the molecular ion peak is confirmed on the PI mass spectrum, the isotope ratio match score is 0.94 (Max:1.00). Thus, each evaluation point showed good results, so the peak at RT 10.04min was judged to be α -Phellandrene.







Fig.4 Result window of Target Analysis

Conclusion

We analyzed the optional aromatic components of herbs and spices from the measurement data of volatile organic compounds of hamburger using target analysis. As a result, the presence of the target components can be confirmed, and it was shown that the target compounds can be analyzed quickly and accurately by "Target Analysis".

1) M. Ubukata et al, Rapid Commun Mass Spectrum., 34 (2020). DOI: 10.1002/rcm.8820 Certain products in this brochure are controlled under the "Foreign Exchange and Foreign Trade Law" of Japan in compliance with international security export control. JEOL Ltd. must provide the Japanese Government with "End-user's Statement of Assurance" and "End-use Certificate" in order to obtain the export license needed for export from Japan. If the product to be exported is in this category, the end user will be asked to fill in these certificate forms.



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