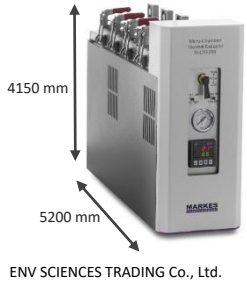
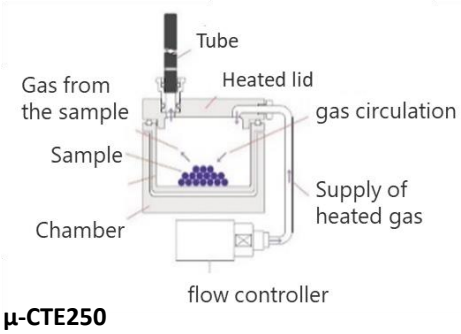
Hamburger Aroma Components Analysis Using Microchamber and Thermal Desorption GC-MS

Product used：Mass Spectrometer (MS)

1. Introduction

The microchamber/heated extraction device is used to collect volatile organic compounds from samples heated in the chamber by a sample tube containing adsorbent. Samples can be placed directly into the chamber and a wide range of sample volumes can be set. Thermal Desorption (TD) is a pretreatment device that heats the sample tube and introduces the desorbed gas into the GC. The gas desorbed from the sample tube is trapped in a cooled focusing trap and then desorbed by rapid heating of the focusing trap. The two-stage thermal desorption system provides high analytical sensitivity. These methods are used in a wide range of fields such as food, fibres, plastics and wood products because of their ability to collect volatile compounds efficiently. (MSTips No.435, 436, 459)In this report we show the useful results of the analysis of food aroma compounds using this method.





μ-CTE250

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

2. Experiment

The sampling procedure is shown in Figure 1. A commercial hamburger weighing 7.5 g was used as the sample. The sample including all ingredients (bun, patty, sauces, pickles) was placed in the microchamber (μ-CTE250, MARKES International Ltd.) lined with aluminum foil. The temperature of the chamber was set at 30 ℃, which is assumed to be the temperature at which the food is consumed. The measurement was performed using a GC-MS (JMS-Q1600GC, JEOL Ltd.) attached to a TD pre-treatment device (TD-Xr100, MARKES International Ltd.). The ionization methods used were electron ionization (EI) and photoionization (PI) as soft ionization (SI). The analysis of the obtained data was performed using the software "Integrated Qualitative Analysis1) " (hereafter referred to as msFineAnalysis iQ) from JEOL Ltd. The measurement conditions are shown in Table 1.

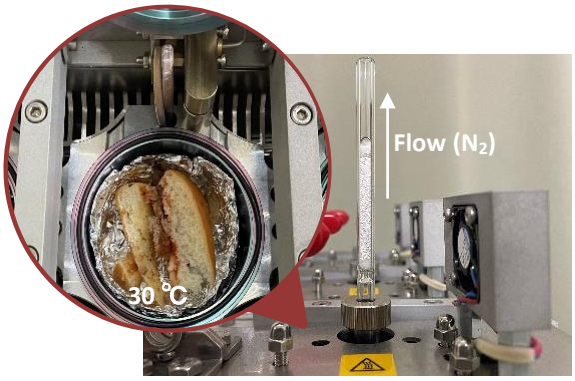


Fig.1 Sampling process

Table 1 Measurement Conditions

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

3. Results

3.1 TICC and Deconvolution peaks

The TICC and deconvolution peaks from the TD-GC-MS measurement are shown in Fig. 2. The deconvolution detection function of msFineAnalysis iQ can identify multiple components in a peak that appears to be a single component, as well as small amounts of components that cannot be detected in the TICC. This function detected 50 peaks (ID:[001]-[050]) in the measurement results.

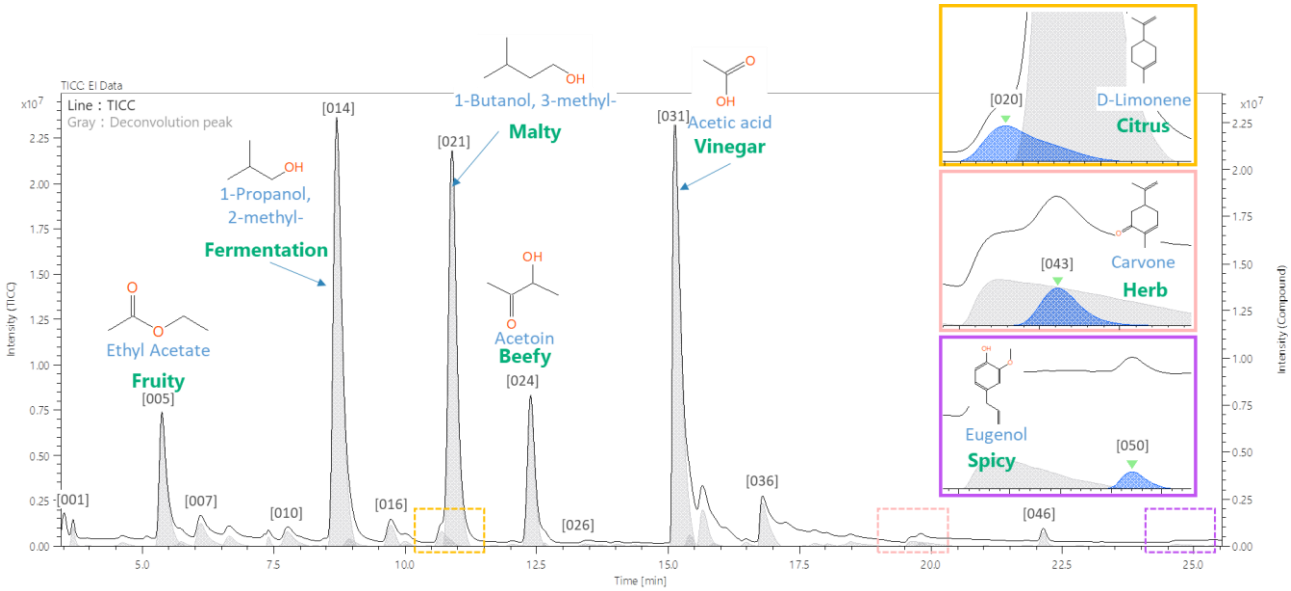


Fig.2 TIC chromatogram and Deconvolution peaks

The main aroma compounds detected were acetic acid from vinegar (sauces, pickles), Acetoin from beef (patties) and 1-Butanol, 3-methyl from malt (buns). In addition, aroma compounds such as D-Limonene, Carvone and Eugenol were detected from citrus fruits, herbs and spices.

3.2 Results of msFineAnalysis iQ

The msFineAnalysis iQ" provides high quality results through integrated qualitative analysis using identification functions such as confirmation of molecular ions in EI and PI data, retention index (RI) and isotope ratio matching in addition to database searching of EI data. In addition, the background color of the table indicates the accuracy of the results, with blue indicating a highly accurate result. As a result, several aroma components suspected to be from hamburger were confirmed with high accuracy.

Table 2 msFineAnalysis iQ results

General			Total Result									Spectrum Info
ID	RT [min]	Height [%]	Library Name	CAS#	Match Factor	ΔRI [iu]	Formula	MW	Molecular Weight Check	Adduct/ Loss	Isotope Matching	IM Ionization
001	3.68	4.31	n-Hexane	110-54-3	930	8	C6 H14	86	✔	none	0.98	SI
002	3.95	0.21	Heptane	142-82-5	756	12	C7 H16	100	✔	none	N/A	EI
003	4.50	0.13	Octane	111-65-9	687	0	C8 H18	114	✔	-C2H5	N/A	EI
004	4.62	0.84	Propanal, 2-methyl-	78-84-2	828	9	C4 H8 O	72	✔	none	0.97	SI
005	5.37	29.94	Ethyl Acetate	141-78-6	941	5	C4 H8 O2	88	✔	none	0.92	SI
006	5.74	1.03	Butanal, 3-methyl-	590-86-3	760	6	C5 H10 O	86	✔	none	N/A	EI
007	6.11	5.27	Ethanol	64-17-5	852	4	C2 H6 O	46	✔	none	0.96	EI
008	6.65	2.34	2,3-Butanedione	431-03-8	852	9	C4 H6 O2	86	✔	none	0.96	SI
009	7.40	2.19	α-Pinene	80-56-8	649	11	C10 H16	136	✔	none	N/A	SI
010	7.76	3.33	1-Propanol	71-23-8	844	1	C3 H8 O	60	✔	none	0.83	SI
011	8.03	0.22	2,3-Pentanedione	600-14-6	776	9	C5 H8 O2	100	✔	none	N/A	SI
012	8.29	0.10	Disulfide, dimethyl	624-92-0	879	14	C2 H6 S2	94	✔	none	N/A	SI
013	8.46	0.17	Hexanal	66-25-1	752	10	C6 H12 O	100	✔	-H2O	N/A	EI
014	8.70	100.00	1-Propanol, 2-methyl-	78-83-1	877	7	C4 H10 O	74	✔	none	0.98	SI
015	8.94	1.66	β-Pinene	127-91-3	868	14	C10 H16	136	✔	none	0.93	SI
016	9.72	4.85	3-Carene	13466-78-9	903	9	C10 H16	136	✔	none	0.95	SI
017	9.99	1.14	Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)-	28634-89-1	815	35	C10 H16	136	-	-	-	SI
018	10.04	0.26	α-Phellandrene	99-83-2	807	13	C10 H16	136	✔	none	N/A	SI
019	10.45	0.08	Heptanal	111-71-7	687	10	C7 H14 O	114	-	-	-	EI
020	10.69	3.39	D-Limonene	5989-27-5	893	4	C10 H16	136	✔	none	0.95	SI
021	10.89	92.83	1-Butanol, 3-methyl-	123-51-3	926	11	C5 H12 O	88	✔	-H2O	0.86	SI
022	11.68	0.19	1-Pyrrolidinamine, N-ethylidene-	60144-27-6	609	0	C6 H12 N2	112	✔	none	N/A	SI
023	12.04	0.42	p-Cymene	99-87-6	835	14	C10 H14	134	✔	none	0.87	SI
024	12.39	34.41	Acetoin	513-86-0	890	9	C4 H8 O2	88	✔	none	0.96	SI
025	12.66	0.71	2-Propanone, 1-hydroxy-	116-09-6	798	12	C3 H6 O2	74	✔	none	N/A	SI
026	13.42	0.55	2-Butanol, 1-methoxy-	53778-73-7	732	9	C5 H12 O2	104	✔	-C2H5	N/A	EI
027	13.55	0.36	1-Hexanol	111-27-3	638	15	C6 H14 O	102	✔	-H2O	N/A	EI
028	13.71	0.29	2-Hydroxy-3-pentanone	5704-20-1	674	17	C5 H10 O2	102	-	-	-	EI
029	14.03	0.45	1-Propanol, 3-ethoxy-	111-35-3	728	6	C5 H12 O2	104	-	-	-	SI
030	14.38	0.22	Nonanal	124-19-6	839	4	C9 H18 O	142	-	-	-	EI
031	15.12	98.58	Acetic acid	64-19-7	916	19	C2 H4 O2	60	✔	none	0.97	EI
032	15.40	2.66	Furfural	98-01-1	941	14	C5 H4 O2	96	✔	none	0.97	SI
033	15.66	8.32	Acetic acid	64-19-7	900	14	C2 H4 O2	60	✔	none	1.00	EI
034	15.88	0.59	1-Hexanol, 2-ethyl-	104-76-7	865	15	C8 H18 O	130	-	-	-	EI
035	16.48	0.90	S-Benzoyl(thiohydroxylamine)	25740-80-1	631	0	C7 H7 N O S	153	✔	-H	N/A	EI
036	16.79	9.97	Propanoic acid	79-09-4	885	3	C3 H6 O2	74	✔	none	0.94	EI
037	17.58	0.08	2,3-Butanediol, [R-(R*,R*)]-	24347-58-8	700	27	C4 H10 O2	90	-	-	-	EI
038	17.80	0.66	Caryophyllene	87-44-5	838	1	C15 H24	204	✔	none	N/A	SI
039	18.03	0.55	Ethanol, 2-(2-ethoxyethoxy)-	111-90-0	871	5	C6 H14 O3	134	-	-	-	SI
040	18.48	1.02	2-Furanmethanol	98-00-0	628	19	C5 H6 O2	98	✔	none	0.80	SI
041	19.41	0.06	1-Propanol, 3-(methylthio)-	505-10-2	703	15	C4 H10 O S	106	✔	none	N/A	SI
042	19.62	1.08	Pentanoic acid	109-52-4	825	14	C5 H10 O2	102	-	-	-	EI
043	19.81	0.88	Carvone	99-49-0	924	7	C10 H14 O	150	✔	none	N/A	SI
044	21.04	0.11	2-Propanol, 1,1'-oxybis-	110-98-5	849	3	C6 H14 O3	134	-	-	-	EI
045	21.82	0.17	Diethylboric acid, (2-methoxyethyl) ester	-	622	N/A	C7 H17 B O2	144	-	-	-	EI
046	22.14	3.10	Phenylethyl Alcohol	60-12-8	964	7	C8 H10 O	122	✔	none	0.95	SI
047	22.82	0.13	1-Hexene, 3,5-dimethyl-	7423-69-0	658	1108	C8 H16	112	✔	-CH3	N/A	EI
048	23.26	0.09	Phenol	108-95-2	695	15	C6 H6 O	94	✔	none	N/A	SI
049	24.67	0.40	Octanoic acid	124-07-2	749	39	C8 H16 O2	144	-	-	-	EI
050	25.35	0.21	Eugenol	97-53-0	726	13	C10 H12 O2	164	✔	none	N/A	SI

Conclusion

We analyzed the aroma compounds in hamburger using microchamber and TD-GC-MS. As a result, several aroma compounds were identified from the hamburger, demonstrating the usefulness of this method for food aroma analysis.

1) M. Ubukata et al, Rapid Commun Mass Spectrum., 34 (2020). DOI: 10.1002/rcm.8820

JEOL Ltd.
3-1-2 Musashino Akishima Tokyo 196-8558 Japan Sales Division Tel. +81-3-6262-3560 Fax. +81-3-6262-3577
www.jeol.com ISO 9001 • ISO 14001 Certified