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Application Data Sheet

No.103

GC-MS
Gas Chromatograph Mass Spectrometer

Analysis of Metabolites Extracted from Human Embryonic Stem Cells Using GC-MS

Metabolome analysis, a comprehensive analysis of the various metabolites generated as biological functions are maintained, is widely used in disease biomarker searches and other investigations. To conduct these investigations, it is necessary to identify the metabolites contained in biological samples.
This application data sheet introduces the results of identifying metabolites extracted from human embryonic stem (ES) cells utilizing the Smart Metabolites Database, which contains metabolites detected in biological samples, such as blood, urine, and cells.

Analysis Conditions

Embryonic stem cell extracts collected respectively from four dishes (60 mm) were subjected to trimethylsilylation (TMS). For detailed procedures regarding the extraction and derivatization of metabolites from cells, refer to Shimadzu Journal vol.2.The sample were analyzed in Q3 scan mode with the triple quadrupole GCMS-TQ8040 using the conditions shown in Table 1.

Table 1: Analysis Conditions

GC-MS:	GCMS-TQ8040
Column:	DB-5 (Length 30 m; 0.25 mm I.D.; df = 1.00 μm)
Glass insert:	Splitless insert with wool (P/N: 221-48876-03)

[GC]	
Sample injection unit temp.:	280 °C
Column oven temp.:	100 °C (4 min) → (4 °C/min) → 320 °C (8 min)
Injection mode:	Splitless
Carrier gas control:	Linear velocity (39.0 cm/sec)
Injection volume:	1 μL

[MS]	
Interface temp.:	280 °C
Ion source temp.:	200 °C
Data acquisition time:	4 min to 67 min
Measurement mode:	Scan
Mass range:	*m/z* 45-600
Event time:	0.3 sec

Analysis Results

Figure 1 shows the resulting total ion current chromatogram (TIC), and Table 2 lists the metabolites identified. From the human ES cell extract, it was possible to identify 124 TMS derivatized metabolites including 2-isopropylmalic acid, added as an internal standard.

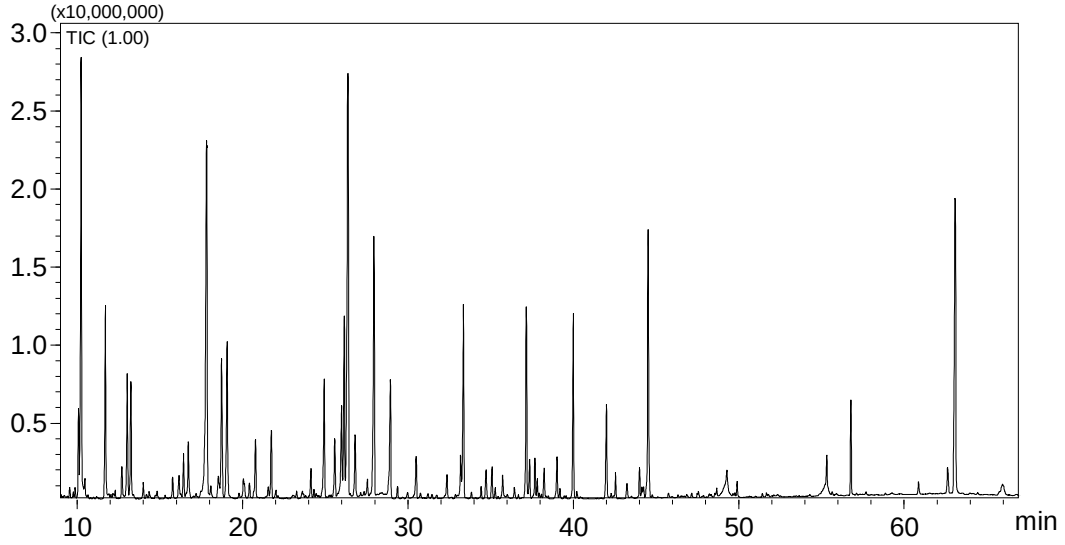

Fig. 1: Total Ion Current Chromatogram (TIC) for Metabolic Components Contained in Human ES Cell Extract

Table 2: List of TMS Derivatized Metabolites Identified *

1	Adenine-2TMS	43	Glycine-2TMS	85	Octadecanol-TMS
2	Adenosine monophosphate-5TMS	44	Glycine-3TMS	86	Octenedioic acid-2TMS
3	Adenosine-4TMS	45	Glycolic acid-2TMS	87	Oleic acid-TMS
4	Alanine-2TMS	46	Glycyl-Glycine-4TMS	88	O-Phosphoethanolamine-4TMS
5	Allose-meto-5TMS(2)	47	Histidine-3TMS	89	O-Phospho-Serine-4TMS
6	4-Aminobutyric acid-2TMS	48	Homocysteine-3TMS	90	Ornithine-3TMS
7	4-Aminobutyric acid-3TMS	49	2-Hydroxyadipic acid-3TMS	91	Ornithine-4TMS
8	3-Aminopropanoic acid-3TMS	50	3-Hydroxybutyric acid-2TMS	92	Oxalic acid-2TMS
9	Arachidonic acid-TMS	51	2-Hydroxyglutaric acid-3TMS	93	5-Oxoproline-2TMS
10	Arginine-3TMS	52	3-Hydroxyglutaric acid-3TMS	94	Palmitic acid-TMS
11	Ascorbic acid-4TMS	53	2-Hydroxyisobutyric acid-2TMS	95	Palmitoleic acid-TMS
12	Asparagine-3TMS	54	3-Hydroxyisobutyric acid-2TMS	96	Pantothenic acid-3TMS
13	Aspartic acid-3TMS	55	3-Hydroxypropionic acid-2TMS	97	Phenylalanine-2TMS
14	Benzoic acid-TMS	56	Hypotaurine-3TMS	98	Phosphoenolpyruvic acid-3TMS
15	Cholesterol-TMS	57	Inositol phosphate-7TMS	99	3-Phosphoglyceric acid-4TMS
16	Citric acid-4TMS	58	Inositol-6TMS(2)	100	Phosphoric acid-3TMS
17	Cystamine-nTMS	59	Isocitric acid-4TMS	101	Proline-2TMS
18	Cystathionine-4TMS	60	2-Isopropylmalic acid-3TMS	102	Putrescine-4TMS
19	Cysteine-3TMS	61	2-Ketoglutaric acid-meto-2TMS	103	Pyridoxine-3TMS
20	Dihydroxyacetone phosphate-meto-3TMS(1)	62	Kynurenine-3TMS	104	Pyruvic acid-meto-TMS
21	Dihydroxyacetone phosphate-meto-3TMS(2)	63	Lactic acid-2TMS	105	Ribitol-5TMS
22	Elaidic acid-TMS	64	Lauric acid-TMS	106	Ribonic acid-5TMS
23	Erythrulose-meto-3TMS(1)	65	Leucine-2TMS	107	Ribose-4TMS(2)
24	Fructose 1-phosphate-meto-6TMS(1)	66	Lysine-4TMS	108	Ribulose 5-phosphate-meto-5TMS(1)
25	Fructose 6-phosphate-meto-6TMS	67	Maleic acid-2TMS	109	Saccharopine-4TMS
26	Fructose-meto-5TMS(2)	68	Malic acid-3TMS	110	Serine-3TMS
27	Fumaric acid-2TMS	69	Mannose 6-phosphate-meto-6TMS(1)	111	Sorbitol-6TMS
28	Galacturonic acid-5TMS(2)	70	Mannose 6-phosphate-meto-6TMS(2)	112	Sorbose-meto-5TMS(1)
29	Galacturonic acid-meto-5TMS(1)	71	Mannose-5TMS(1)	113	Stearic acid-TMS
30	Galacturonic acid-meto-5TMS(2)	72	Mannose-meto-5TMS(2)	114	Succinic acid-2TMS
31	Glucaric acid-6TMS	73	Margaric acid-TMS	115	Threonic acid-4TMS
32	Glucose 6-phosphate-meto-6TMS(1)	74	Methionine-2TMS	116	Threonine-3TMS
33	Glucose-5TMS(2)	75	3-Methylglutaconic acid(Z)-2TMS	117	Thymine-2TMS
34	Glucose-meto-5TMS(1)	76	7-Methylguanine-2TMS	118	Trehalose-8TMS
35	Glucose-meto-5TMS(2)	77	Monostearin-2TMS	119	Tyrosine-3TMS
36	Glucuronic acid lactone-3TMS(2)	78	Myristic acid-TMS	120	Urea-2TMS
37	Glucuronic acid-meto-5TMS(1)	79	N-Acetylaspartic acid-2TMS	121	Ureidosuccinic acid-3TMS
38	Glutamic acid-3TMS	80	N-Acetylaspartic acid-3TMS	122	Valine-2TMS
39	Glutamine-3TMS	81	N-Acetylglutamine-3TMS	123	Xylitol-5TMS
40	Glutamine-4TMS	82	N-Acetylmannosamine-meto-4TMS(2)	124	Xylulose-meto-4TMS
41	Glycerol 3-phosphate-4TMS	83	Niacinamide-TMS		
42	Glycerol-3TMS	84	Nonanoic acid-TMS		

* : TMS and meto indicate trimethylsilylation and methoximation, respectively.

Note: The human ES cells were provided by Dr. Kazuhiro Aiba and Prof. Norio Nakatsuji, Institute for Integrated Cell-Material Sciences, Kyoto University.

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