

Supplementary Materials

Sustainable Development of Dairy-Based Functional Beverages Enriched with Bee Pollen: A Circular Economy Approach

Table S1. Volatile compounds (relative content, %) in fermented dairy beverages samples.

No	Compounds	Flavor description ²	CAS	RI _{cal} ³	RI _{ref} ⁴	MB37.5	MW37.5	MW75	MBW	M100	MB75
Esters											
1	Ethyl acetate	Pineapple	141-78-6	-	878	1.56	4.25	1.79	3.55	1.68	4.76
2	Vinyl acetate		108-05-4	988	-	0.43	0.59	0.40	0.75	0.59	1.23
3	Methyl butanoate	Ether Fruity Sweet	623-42-7	993	989	0.14	0.20	0.09	0.30	0.10	0.29
4	Isobutyl acetate	Fruity Apple Banana	110-19-0	1019	1018	1.34	3.37	1.92	2.96	1.36	3.81
5	Ethyl butyrate	Apple	105-54-4	1041	1042	0.43	0.34	0.31	0.19	-	0.23
6	2-Pentyl acetate	Herbaceous	626-38-0	1078	1075	3.76	8.73	5.72	8.53	9.11	10.32
7	Isobutyl isobutyrate	Pineapple	97-85-8	1094	1092	0.61	0.09	0.23	0.11	0.07	0.07
8	Isoamyl acetate	Banana	123-92-2	1126	1125	4.51	14.41	9.55	10.66	6.21	13.68

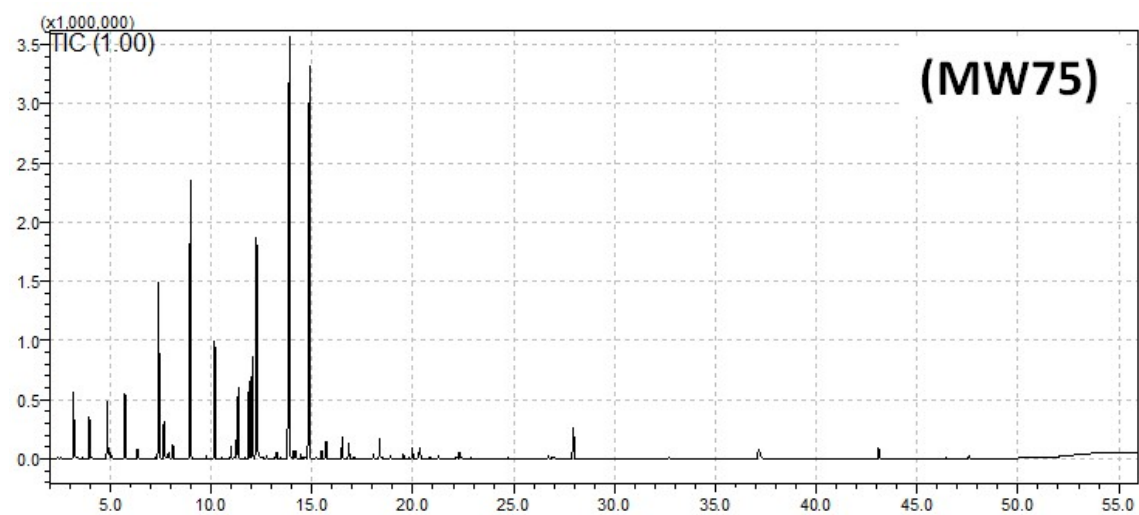
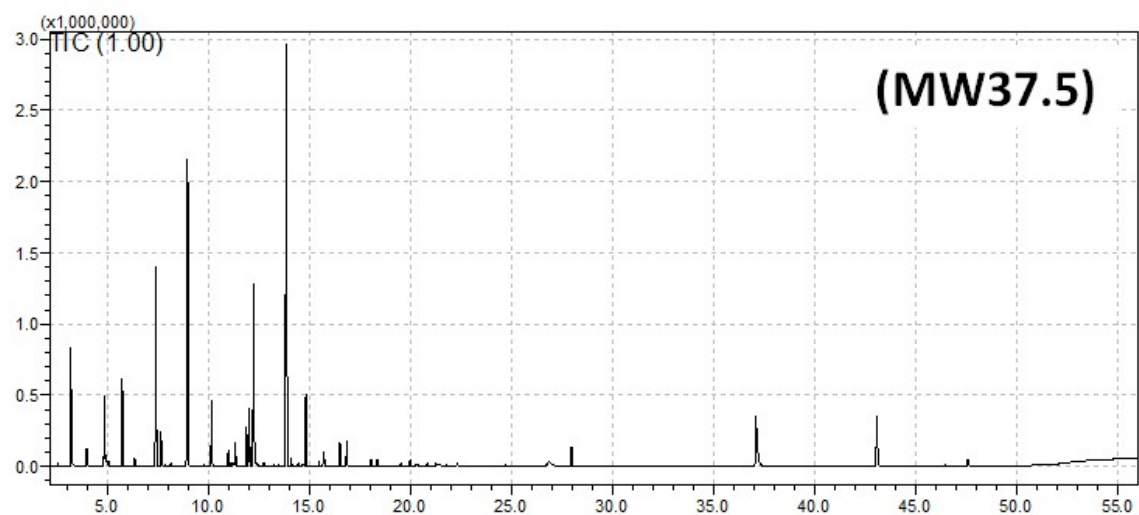
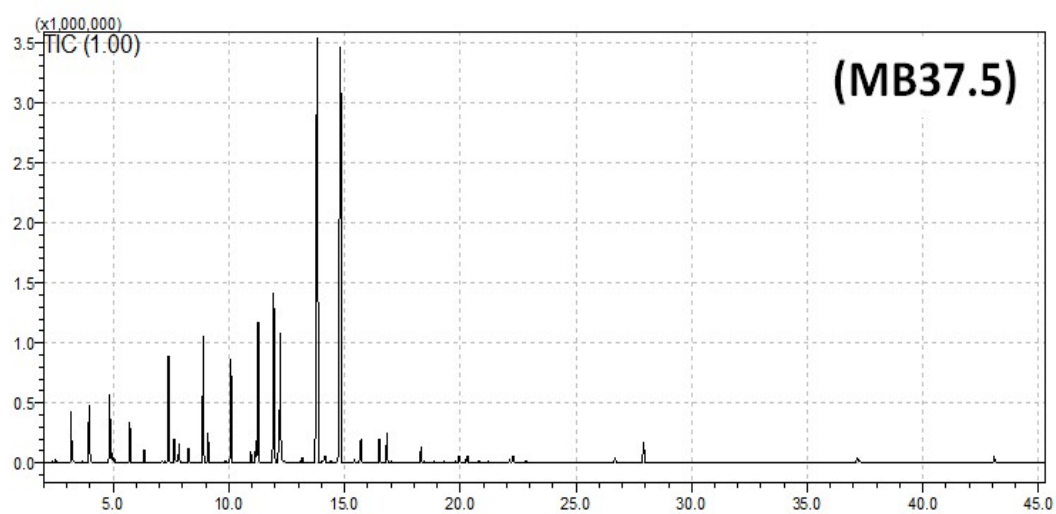
9	Isobutyl butyrate	Sweet Fruity Apple Pineapple	539-90-2	1162	1160	3.65	2.68	3.66	3.07	4.21	1.88
10	Isobutyl isovalerate		589-59-3	1194	1191	0.92	0.12	0.66	0.14	0.14	-
11	Isoamyl isobutyrate	Fruity	2050-01-3	1197	1195	5.20	0.99	2.21	1.04	0.77	0.57
12	Propanoic acid, 2- methyl-, 1- methylbutyl ester		54340-93-1	1219	-	0.47	2.55	3.86	3.71	9.23	2.42
13	Ethyl hexanoate	Apple Fruity	123-66-0	1240	1236	-	0.15	0.10	-	-	-
14	Butyl isovalerate	Fruity	109-19-3	1253	1250	0.23	-	0.19	-	-	-
15	Isoamyl butyrate	Fruity banana	106-27-4	1272	1267	25.70	24.11	25.35	23.82	27.36	16.97
16	Hexyl acetate	Fruity Herb	142-92-7	1278	1275	0.12	0.37	0.29	0.31	-	-
17	Isoamyl 2- methylbutyrate	Fruity	27625-35-0	1281	1274	0.26	-	0.25	0.06	-	-

18	Prenyl isobutyrate	Fruity Buttery	76649-23-5	1289	-	0.09	0.13	0.14	0.15	0.28	-
19	Isoamyl isovalerate	Fruity Apple	659-70-1	1301	1294	22.96	2.96	17.67	3.04	2.68	2.19
20	Methyl octanoate	Orange	111-11-5	1397	1390	-	0.29	0.12	0.13	-	-
21	Butanoic acid, 1- methylhexyl ester		39026-94-3	1405	1401	0.56	0.31	0.63	0.40	0.86	0.50
Alcohols											
22	Ethanol	Sweet	64-17-5	938	937	2.13	0.84	1.31	0.91	0.59	1.04
23	Isobutanol	Wine Solvent Bitter	78-83-1	1107	1108	0.59	0.18	0.46	0.29	0.13	0.35
24	2-pentanol	Green	6032-29-7	1132	1127	0.95	-	-	-	-	-
25	Butanol	Medicine Fruity	71-36-3	1155	1157	0.08	0.10	0.09	0.13	0.08	0.13
26	3-Methyl-1- butanol	Whiskey Malt Burnt	123-51-3	1217	1217	8.41	1.64	2.36	2.59	1.11	3.19
27	2-heptanol	Mushroom	543-49-7	1327	1326	0.92	0.67	0.61	1.12	1.10	1.59

28	Hexanol	Resin Flower Green	111-27-3	1361	1362	1.01	1.05	0.54	1.19	0.67	1.56
Ketones											
29	2-pentanone	Ether Wine Fruity	107-87-9	983	982	2.30	2.73	1.66	4.64	3.68	5.55
30	2-heptanone	Soap	110-43-0	1188	1188	0.43	0.67	0.37	0.95	0.93	0.96
Aldehydes											
31	Hexanal	Grass Tallow Fat	66-25-1	1087	1087	0.78	1.64	1.35	2.74	3.56	2.49
32	2-hexenal, (E)-	Apple Green Vegetable	6728-26-3	1225	1220	4.77	9.68	9.55	12.08	15.79	12.31
Ether											
33	Butane, 1-methoxy-3-methyl-		626-91-5	1351	-	0.84	0.96	0.67	1.37	1.35	2.01
Acids											

34	Hexanoic acid	Sweat	142-62-1	-	1849	0.40	5.10	0.76	2.94	0.64	2.80
35	Octanoic acid	Sweat, Cheese	124-07-2	-	2038	0.32	3.08	0.52	1.75	0.41	1.82

¹ Flavor description were checking from the Specifications for Flavourings presented by JECFA (Joint FAO/WHO Expert Committee on Food Additives) (<https://www.fao.org/food-safety/scientific-advice/jecfa/en/>), and Flavor Substances website (<https://www.flavornet.org/>); ² RI_{cal} is the retention index value calculated according to eqn (4); ³ RI_{ref} is the reference retention index value consulted on the website (<https://webbook.nist.gov/chemistry/>); and “-” Information not available. The chromatograms are presented in Fig. S1 in the Supplementary Material.



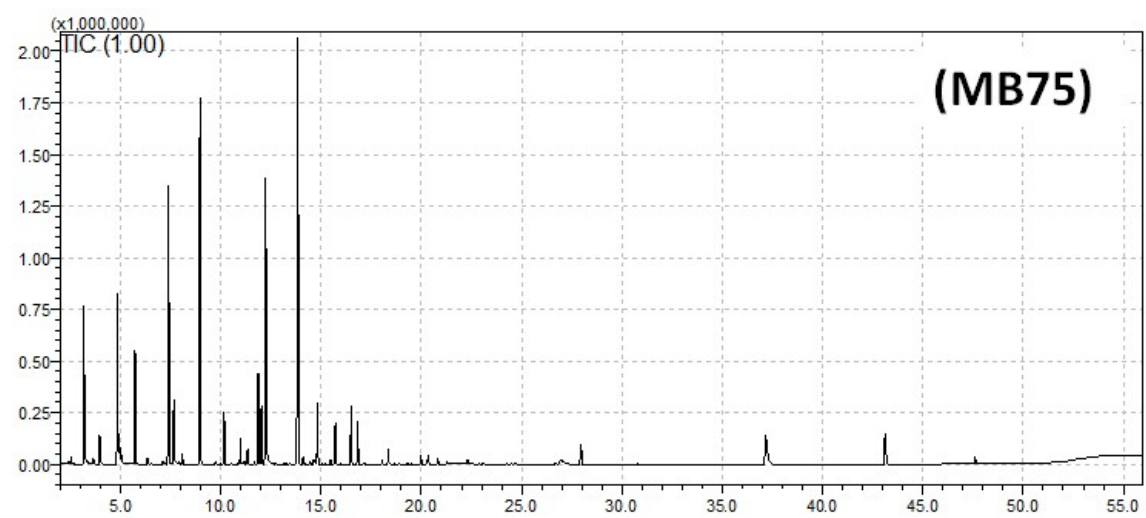
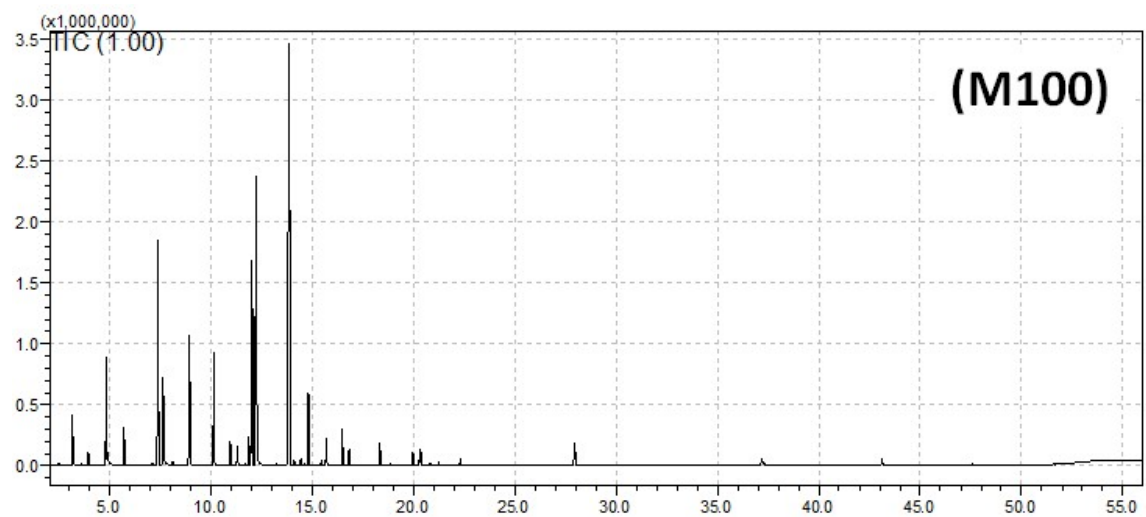
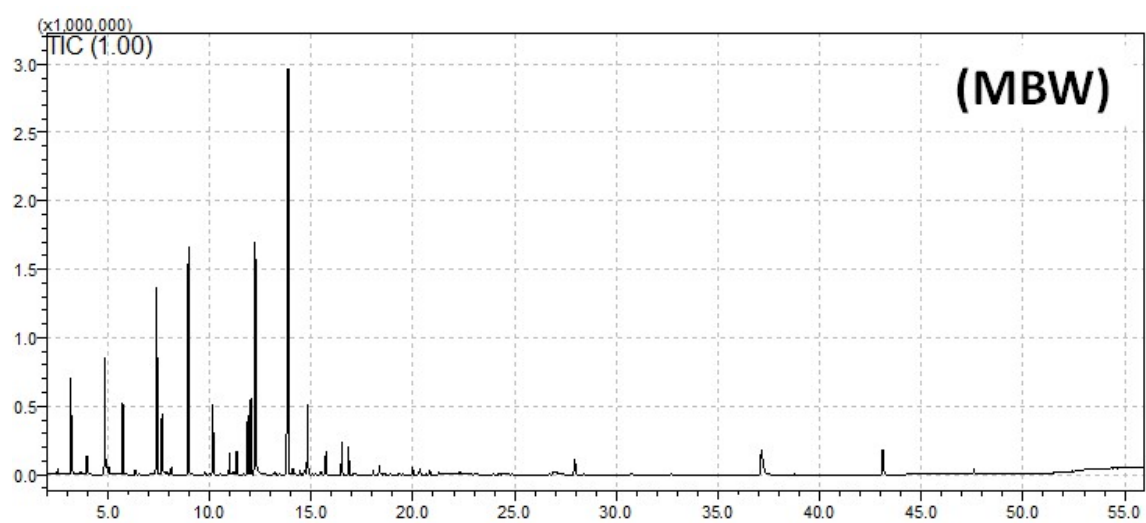


Fig. S1 Chromatograms obtained from the analysis of samples of fermented dairy beverages by gas chromatography coupled to mass spectrometry (GC-MS).