

Supporting information

Table S1. The entire milk volatile organic compound profile according to the retention time (RT, min)

RT	Assignment	Chemical class	Formula	Molecular weight
1.43	Isobutyraldehyde	ALDEHYDE	C ₄ H ₈ O	72.11
1.50	Isopropyl alcohol; Isopropanol	ALCOHOL	C ₃ H ₈ O	60.10
1.56	Diacetyl	KETONE	C ₄ H ₆ O ₂	86.09
1.61	Hexane	ALKANE	C ₆ H ₁₄	86.18
1.62	N/A	-	-	-
1.65	3-Methylbutanal; Isovaleraldehyde	ALDEHYDE	C ₅ H ₁₀ O	86.13
1.72	isobutyl alcohol	ALCOHOL	C ₄ H ₁₀ O	74.123
1.88	Propionic acid, Propanoic acid, Ethylformic acid	CARBOXYLIC ACID	C ₃ H ₆ O ₂	74.08
1.96	2-Pentanol	ALCOHOL	C ₅ H ₁₂ O	88.15
2.09	N/A	-	-	-
2.20	Isobutyric acid	CARBOXYLIC ACID	C ₄ H ₈ O ₂	88.11
2.47	Amyl alcohol, 1-Pentanol	ALCOHOL	C ₅ H ₁₂ O	88.15
2.54	Isobutyl acetate	ESTER	C ₆ H ₁₂ O ₂	116.16
2.64	Methyl-2-methylbutyrate	ESTER	C ₆ H ₁₂ O ₂	116.16
2.81	3,4-Hexanedione	KETONE	C ₆ H ₁₀ O ₂	114.07
3.05	Ethyl lactate	ESTER	C ₅ H ₁₀ O ₃	118.13
3.68	2-Hexen-1-ol (trans)	ALCOHOL	C ₆ H ₁₂ O	100.16
4.17	Valeric acid	CARBOXYLIC ACID	C ₅ H ₁₀ O ₂	102.13
4.25	cis-4-Heptenal	ALDEHYDE	C ₇ H ₁₂ O	112.17
4.35	Ethyl valerate; Ethyl pentanoate	ESTER	C ₇ H ₁₄ O ₂	130.18
4.45	Heptanal	ALDEHYDE	C ₇ H ₁₄ O	114.10
4.77	Isobutyl isobutyrate	ESTER	C ₈ H ₁₆ O ₂	144.21
6.35	Hexanoic acid	CARBOXYLIC ACID	C ₆ H ₁₂ O ₂	117.15
6.51	2-Octanone	KETONE	C ₈ H ₁₆ O	128.215
6.84	2-Octanol	ALCOHOL	C ₈ H ₁₈ O	130.23
7.60	p-Methylanisole	ETHER	C ₈ H ₁₀ O	122.17
7.87	2-Ethyl-1-hexanol	ALCOHOL	C ₈ H ₁₈ O	130.23
8.01	Isopropyl hexanoate	ESTER	C ₉ H ₁₈ O ₂	158.24
9.48	Heptanoic acid	CARBOXYLIC ACID	C ₇ H ₁₄ O ₂	130.19
9.64	Butyl butyrate	ESTER	C ₈ H ₁₆ O ₂	144.21
10.29	Methyl benzoate	ESTER	C ₈ H ₈ O ₂	136.15
11.15	Isophorone; 3, 5, 5-Trimethyl-2-cyclohexen-1-one	KETONE	C ₉ H ₁₄ O	138.21
12.80	alpha,alpha-Dimethylphenethyl acetate	ESTER	C ₁₂ H ₁₆ O ₂	192.26
13.61	Diethyl succinate	ESTER	C ₈ H ₁₄ O ₄	174.20
13.63	Octanoic acid	CARBOXYLIC ACID	C ₈ H ₁₆ O ₂	144.214

15.13	trans,trans-2,4-Nonadienal	ALDEHYDE	C ₉ H ₁₄ O	138.21
16.12	cis-3-Hexenyl isovalerate, Hex-3-enyl isovalerate	ESTER	C ₁₁ H ₂₀ O ₂	184.28
20.39	Anisyl formate	ALDEHYDE	C ₉ H ₁₀ O ₃	166.18
21.95	3-Phenylpropyl acetate	ESTER	C ₁₁ H ₁₄ O ₂	178.23
22.06	Decanoic acid	CARBOXYLIC ACID	C ₁₀ H ₂₀ O ₂	172.27
24.35	trans-Cinnamic acid	CARBOXYLIC ACID	C ₉ H ₈ O ₂	148.16
27.68	N/A	-	-	-
34.59	gamma-Dodecalactone	KETONE	C ₁₂ H ₂₂ O ₂	198.306

N/A, not assigned

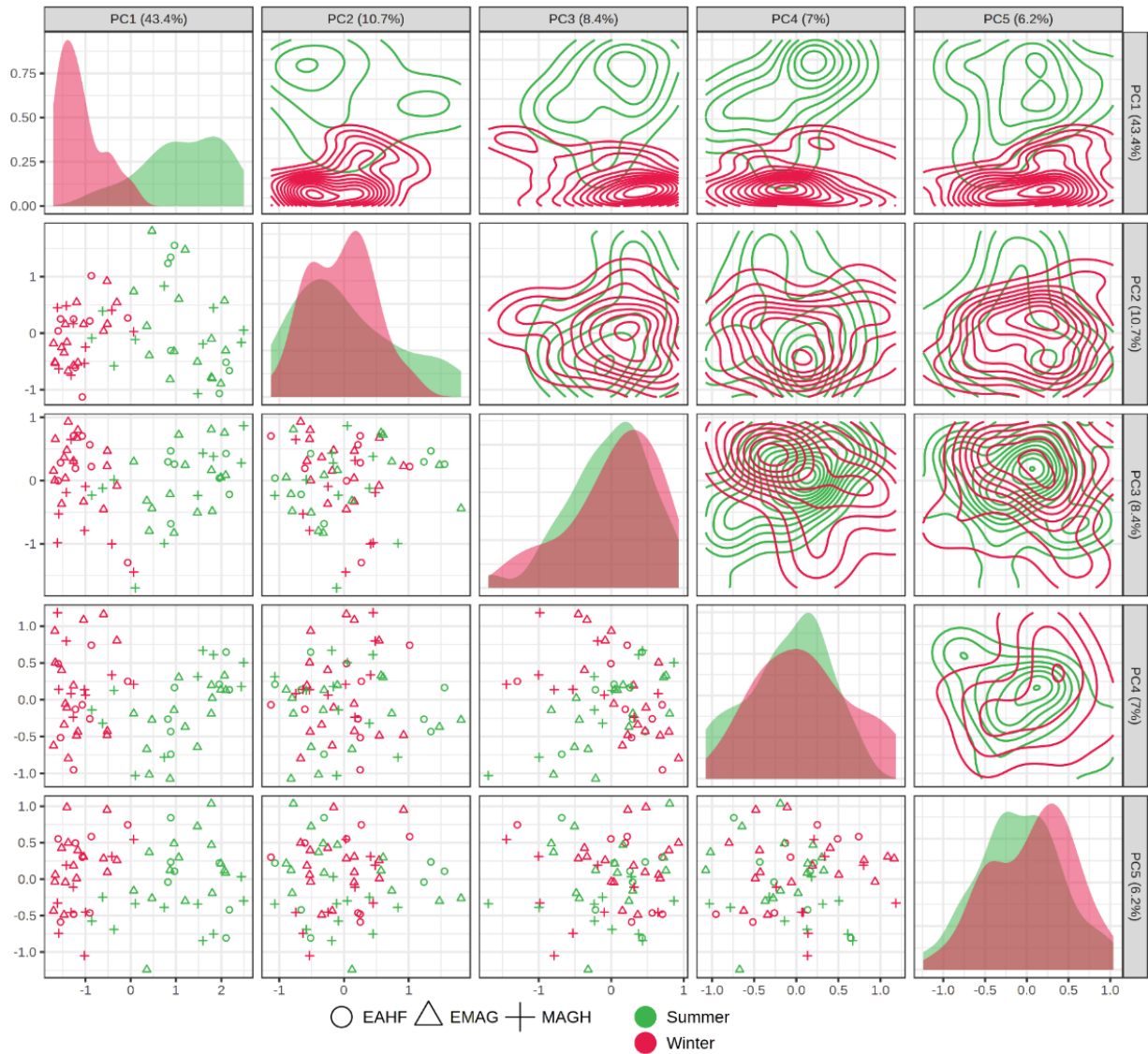


Figure S1. Interactive principal component analysis (iPCA) applied to raw milk VOC profiles according to the feeding systems (EMAG, ensiled maize and grass, Δ ; EAHF, ensiled and haylage forage, \circ ; MAGH, meadow and grass hay, $+$) and seasons (summer, green; winter, red). The principal components PC1 and PC2 explain the 54.3% of total variance. Contribution to the explanation of the variance was provided also by PC1-PC3 and PC1-PC4.