

Supplementary Materials

Table S1: Microbial results for the raw and pasteurized milk samples (grass (GRS), clover (CLV) and total mixed ration (TMR)). VRB: Violet Red Bile, KAA: Kanamycin Aesculin Azide, MPCA: Milk Plate Count Agar.

Table S2: Composition analysis results for pasteurized grass (GRS), clover (CLV) and total mixed ration (TMR) milk samples in early, mid and late lactation. Each result is the average of 2 replicates.

Table S3: Individual Free Fatty Acid Content mg/kg or ppm (relative standard deviation of the results between replicates as a percent in brackets) for each of the pasteurized (p) milk samples (grass (GRS), grass/clover (CLV) and total mixed ration (TMR)) at day 3, 9 and 14 of refrigerated storage. * $p = 0.05$, d = day.

Table S4: Individual Free fatty acid content mg/kg (relative standard deviation of the results between replicates as a percent in brackets) for each of the pasteurized (p) milk samples (grass (GRS), grass/clover (CLV) and total mixed ration (TMR)) at day 3, 9 and 14 of refrigerated storage and the significance between the fatty acids analysed for each sample (GRS, CLV and TMR). * $p = 0.05$, d = day, NS = not significant.

Figure S1: Bar chart showing the levels of important isoflavones in feed samples (grass, grass/clover and total mixed ration (TMR)) and the corresponding raw (r) and pasteurized (p) grass (GRS), clover (CLV) and total mixed ration (TMR) milk samples.

Figure S2: Hierarchical clustering analysis (Heatmap) of the average values for the top 65 volatile organic compounds contributing to the differences between grass, grass/clover and total mixed ration (TMR) feed samples, as determined by headspace solid-phase microextraction gas-chromatography mass spectrometry (HS-SPME GC-MS) analysis. Positive and negative correlations between feeding system (grass, grass/clover and TMR) and volatile organic compounds is denoted by +1 (red) and -1 (blue).

Figure S3: Bar charts showing the percentage of each chemical class (aldehydes, ketones, alcohols, acids, fatty acid esters, terpenes, furans, hydrocarbons, sulphurs, lactones, pyrazines, ether and phenol) identified in each feed type (grass, grass/clover and total mixed ration (TMR)). 90, 104 and 94 compounds were identified in grass, grass/clover and TMR feeds, respectively.

Table S5: Relationship between cow diet (grass, grass/clover and total mixed ration (TMR)) and the pasteurized (p) milk volatile compounds identified by HS SPME GC-MS at day 3, 9 and 14 of refrigerated storage; values are expressed as peak area values for each compound; values are expressed as peak area values for each compound. d = day, * $p = 0.05$, ND = not detected, NS = not significant.

Table S6: The 26 sensory descriptors used for the evaluation of the 3 pasteurized milk samples (grass (GRS), clover (CLV) and total mixed ration (TMR)) by full descriptive sensory analysis.

Table S1. Microbial results for the raw and pasteurized milk samples (grass (GRS), clover (CLV) and total mixed ration (TMR)). VRB: Violet Red Bile, KAA: Kanamycin Aesculin Azide, MPCA: Milk Plate Count Agar.

		Raw Milk			Pasteurized Milk			
		Agar Type	GRS	CLV	TMR	GRS	CLV	TMR
Early lactation		VRB agar	0.0	1.5	0.0	0.0	0.0	0.0
	Bacteria count (Log ₁₀)	KAA agar	1.0	0.7	1.9	0.7	0.7	1.0
		MPCA	0.0	0.0	0.0	0.0	0.0	0.0
Mid lactation		VRB agar	0.0	0.0	1.4	0.0	0.0	0.0
	Bacteria count (Log ₁₀)	KAA agar	1.0	1.0	1.7	0.0	0.0	0.0
		MPCA	2.0	0.0	2.3	0.0	0.0	0.0
Late lactation		VRB agar	1.0	1.5	3.8	0.0	0.0	0.0
	Bacteria count (Log ₁₀)	KAA agar	0.0	1.7	2.4	0.0	0.0	0.0
		MPCA	0.0	0.0	0.0	0.0	0.0	0.0

Table S2. Monthly averages of composition analysis for pasteurized milk samples from cows on different feeding systems; perennial ryegrass (GRS), perennial ryegrass/white clover (CLV) and total mixed ration (TMR) during mid and late lactation.

Component	Diet	Mid Lactation		Late Lactation		<i>p</i> -Value
		May	June	September	October	
Fat %	GRS	3.4	3.7	2.7	2.8	<0.001
	CLV	3.4	3.4	5.1	4.7	
	TMR	4.2	3.9	2.2	4.4	
Protein %	GRS	3.5	3.6	4.0	3.6	<0.001
	CLV	3.6	3.6	4.1	3.8	
	TMR	3.2	3.4	3.9	3.7	
Lactose %	GRS	4.8	4.7	4.8	4.3	<0.001
	CLV	5.0	4.7	4.8	4.6	
	TMR	4.8	4.7	5.0	4.7	
True protein %	GRS	3.3	3.4	3.8	3.4	<0.001
	CLV	3.4	3.5	3.9	3.6	
	TMR	3.1	3.2	3.7	3.5	
Casein %	GRS	2.7	2.7	3.1	2.7	<0.001
	CLV	2.7	2.8	3.2	2.9	
	TMR	2.4	3.2	3.7	2.9	

Table S3. Individual Free Fatty Acid Content mg/kg or ppm (relative standard deviation of the results between replicates as a percent in brackets) for each of the pasteurized (p) milk samples (grass (GRS) grass/clover (CLV) and total mixed ration (TMR)) at day 3, 9 and 14 of refrigerated storage. * $p = 0.05$, d = day.

Fatty Acid	Grass d 3	Grass/Clover d 3	TMR d 3	Grass d 9	Grass/Clover d 9	Grass d 14	Grass/Clover d 14	TMR d 14	<i>p</i> -Value
C4	3.0 (41.3)	0.0 (0)	0.0 (0)	3.9 (11.9)	8.5 (11)	0.0 (0)	0.0 (0)	0.0 (0)	*
C6	4.4 (4.7)	2.4 (17.1)	2.3 (2.8)	5.3 (2.9)	8.2 (5.2)	6.9 (32.9)	6.4 (14.4)	5.6 (17.3)	*
C8	4.2 (4.9)	2.3 (18.5)	2.5 (4.8)	6.0 (0.1)	8.9 (4)	7.6 (32.2)	6.8 (14.3)	6.1 (18.4)	*
C10	7.5 (7)	4.3 (15.3)	5.1 (22.2)	11.3 (0.2)	16.7 (3.7)	14.7 (31.7)	12.9 (14.9)	12.0 (17.9)	*
C12	8.7 (4.1)	4.9 (15.2)	6.9 (19.5)	12.9 (0.7)	18.7 (2.7)	16.4 (26.2)	13.6 (9.1)	15.0 (16.9)	*
C14	15.9 (7.4)	10.2 (16)	10.6 (14.3)	24.3 (0.3)	38.1 (2.8)	33.3 (25.5)	28.1 (6.1)	29.2 (14.8)	*
C16	67.4 (5.5)	48.9 (13.8)	51.1 (4.1)	88.2 (2.5)	130.8 (2.6)	122.8 (19.6)	91.6 (2.5)	111.8 (8.5)	*
C18	38.7 (6.3)	26.7 (22.3)	30.0 (1.8)	45.5 (3.1)	56.8 (2.7)	58.7 (14.9)	42.6 (3.4)	47.6 (4.6)	*
C18:1	27.1 (4.2)	20.1 (36.4)	14.4 (3.1)	63.9 (1)	92.8 (0.5)	99.9 (24.3)	78.4 (10.6)	87.0 (10.2)	*
C18:2	3.2 (5.7)	2.8 (55.1)	3.6 (29.9)	5.8 (3.8)	8.2 (12.4)	8.8 (27.9)	8.2 (12.2)	10.1 (24.4)	*
C18:3	3.7 (1.3)	1.5 (44.7)	4.1 (20.8)	6.2 (6.7)	7.2 (4.3)	5.0 (22.1)	6.0 (2.4)	2.2 (24.3)	*
Result Total	183.7 (4.7)	124.1 (21.1)	130.6 (6.1)	273.3 (1.5)	394.8 (2)	374 (22.1)	294.5 (6.8)	326.7 (10.6)	*

Table S4. Individual Free fatty acid content mg/kg (relative standard deviation of the results between replicates as a percent in brackets) for each of the pasteurized (p) milk samples (grass (GRS), grass/clover (CLV) and total mixed ration (TMR)) at day 3, 9 and 14 of refrigerated storage and the significance between the fatty acids analyzed for each sample (GRS, CLV and TMR). * $p = 0.05$, d = day, NS = not significant.

Fatty Acid	Grass d 3	Grass d 9	Grass d 14	<i>p</i> -Value	Grass/Clover d 3	Grass/Clover d 9	Grass/Clover d 14	<i>p</i> -Value	TMR d 3	TMR d 14	<i>p</i> -Value
C4	3.0 (41.3)	3.9 (11.9)	0.0 (0)	*	0.0 (0)	8.5 (11)	0.0 (0)	*	0.0 (0)	0.0 (0)	NS
C6	4.4 (4.7)	5.3 (2.9)	6.9 (32.9)	NS	2.4 (17.1)	8.2 (5.2)	6.4 (14.4)	*	2.3 (2.8)	5.6 (17.3)	*
C8	4.2 (4.9)	6.0 (0.1)	7.6 (32.2)	NS	2.3 (18.5)	8.9 (4)	6.8 (14.3)	*	2.5 (4.8)	6.1 (18.4)	*
C10	7.5 (7)	11.3 (0.2)	14.7 (31.7)	NS	4.3 (15.3)	16.7 (3.7)	12.9 (14.9)	*	5.1 (22.2)	12.0 (17.9)	NS
C12	8.7 (4.1)	12.9 (0.7)	16.4 (26.2)	NS	4.9 (15.2)	18.7 (2.7)	13.6 (9.1)	*	6.9 (19.5)	15.0 (16.9)	NS
C14	15.9 (7.4)	24.3 (0.3)	33.3 (25.5)	NS	10.2 (16)	38.1 (2.8)	28.1 (6.1)	*	10.6 (14.3)	29.2 (14.8)	*
C16	67.4 (5.5)	88.2 (2.5)	122.8 (19.6)	NS	48.9 (13.8)	130.8 (2.6)	91.6 (2.5)	*	51.1 (4.1)	111.8 (8.5)	*
C18	38.7 (6.3)	45.5 (3.1)	58.7 (14.9)	NS	26.7 (22.3)	56.8 (2.7)	42.6 (3.4)	*	30.0 (1.8)	47.6 (4.6)	*
C18:1	27.1 (4.2)	63.9 (1)	99.9 (24.3)	*	20.1 (36.4)	92.8 (0.5)	78.4 (10.6)	*	14.4 (3.1)	87.0 (10.2)	*
C18:2	3.2 (5.7)	5.8 (3.8)	8.8 (27.9)	NS	2.8 (55.1)	8.2 (12.4)	8.2 (12.2)	*	3.6 (29.9)	10.1 (24.4)	NS
C18:3	3.7 (1.3)	6.2 (6.7)	5.0 (22.1)	NS	1.5 (44.7)	7.2 (4.3)	6.0 (2.4)	*	4.1 (20.8)	2.2 (24.3)	NS

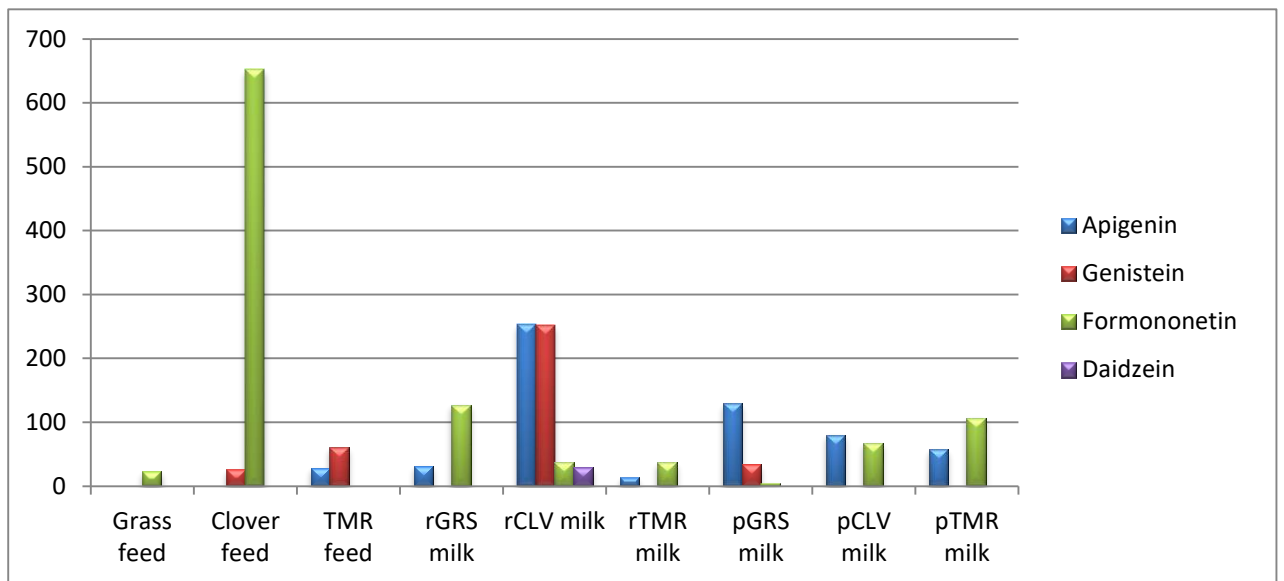


Figure S1. Bar chart showing the levels of important isoflavones in feed samples (grass, clover and total mixed ration (TMR)) and the corresponding raw (r) and pasteurized (p) grass (GRS), clover (CLV) and total mixed ration (TMR) milk samples.

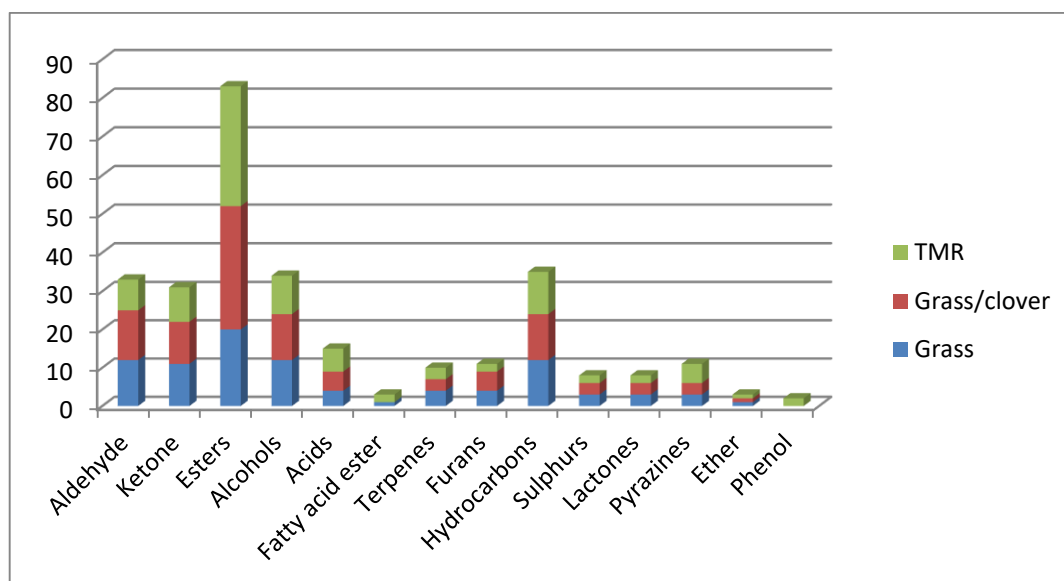


Figure S3. Bar charts showing the percentage of each chemical class (aldehydes, ketones, alcohols, acids, fatty acid esters, terpenes, furans, hydrocarbons, sulphurs, lactones, pyrazines, ether and phenol) identified in each feed type (grass, grass/clover and total mixed ration (TMR)). 90, 104 and 94 compounds were identified in grass, grass/clover and TMR feeds, respectively.

Table S5. Relationship between cow diet (grass, grass/clover and total mixed ration (TMR)) and the pasteurized (p) milk volatile compounds identified by headspace solid-phase microextraction gas-chromatography mass spectrometry (HS-SPME GC-MS) at day 3, 9 and 14 of refrigerated storage; values are expressed as peak area values for each compound; values are expressed as peak area values for each compound. d = day, * $p = 0.05$, ND = not detected, NS = not significant. LRI = Linear retention index.

Compound	CAS No.	LRI	Grass d 3	Grass/Clover d 3	TMR d 3	Grass d 9	Grass/Clo ver d 9	TMR Day 9	Grass Day 14	Grass/Clo ver d 14	TMR Day 14	<i>p</i> -Value	<i>p</i> -Value (Grass)	<i>p</i> -Value (Grass/C lover)	<i>p</i> -Value (TMR)
Aldehyde															
(<i>E</i>)-2-Octenal (or isomer)	2548-87-0	1094	0.00×00	0.00×00	0.00×00	3.80×10^7	0.00×00	5.05×10^8	1.67×10^8	0.00×00	2.20×10^7	*<0.001	NS 0.499	ND	*<0.001
(<i>Z</i>)-2-Heptenal (or isomer)	57266-86-1	1012	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	2.26×10^7	*<0.001	ND	ND	*<0.001
Butanal	123-72-8	627	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	1.31×10^6	0.00×00	1.08×10^7	*<0.001	NS 0.422	ND	*0.001
3-Methyl-butanal	590-86-3	690	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	NS 0.469	NS 0.422	ND	ND
Decanal	112-31-2	1250	8.17×10^6	4.70×10^6	4.45×10^6	1.46×10^7	2.56×10^6	6.46×10^6	1.06×10^7	4.68×10^6	6.58×10^6	NS 0.100	NS 0.470	NS 0.211	NS 0.825
Heptanal	111-71-7	941	2.64×10^8	2.74×10^8	1.33×10^8	1.98×10^8	1.81×10^8	0.00×00	6.35×10^8	2.52×10^8	1.00×10^9	*<0.001	*<0.001	* 0.009	*<0.001
Hexanal	66-25-1	838	3.91×10^8	3.65×10^8	5.35×10^8	2.74×10^8	2.50×10^8	0.00×00	6.33×10^8	2.91×10^8	4.45×10^9	*<0.001	*0.018	*0.031	*<0.001
Nonanal	124-19-6	1147	1.49×10^8	2.31×10^8	1.83×10^8	1.28×10^8	9.04×10^7	4.55×10^7	8.62×10^7	8.08×10^7	1.42×10^8	*<0.001	NS 0.120	*0.009	*<0.001
Octanal	124-13-0	1044	4.97×10^7	6.24×10^7	4.56×10^7	4.54×10^7	3.49×10^7	0.00×00	4.38×10^7	5.88×10^7	1.09×10^8	*<0.001	NS 0.867	*0.012	*<0.001
Pentanal	110-62-3	733	7.14×10^8	7.90×10^8	6.47×10^7	5.25×10^8	7.04×10^8	0.00×00	5.87×10^8	6.29×10^8	2.46×10^8	*<0.001	*0.014	*0.025	*0.018
Ketone															
2-Butanone	78-93-3	637	6.30×10^7	1.04×10^8	1.53×10^8	7.61×10^7	9.97×10^7	8.76×10^7	7.26×10^7	9.84×10^7	1.43×10^8	*0.001	NS 0.868	NS 0.892	*0.001

2-Heptanone	110-43-0	933	3.73×10^7	3.80×10^7	3.18×10^7	1.40×10^8	4.27×10^7	7.14×10^9	6.77×10^8	6.23×10^7	5.85×10^7	*<0.001	NS 0.416	* 0.011	*<0.001
2-Hexanone	591-78-6	831	1.10×10^7	6.07×10^6	4.99×10^6	1.51×10^7	1.15×10^7	6.02×10^7	2.74×10^7	2.49×10^7	1.66×10^7	*<0.001	NS 0.281	* 0.003	*<0.001
2-Nonanone	821-55-6	1137	0.00 × 00	0.00 × 00	0.00 × 00	8.11×10^7	0.00 × 00	2.15×10^9	1.97×10^8	0.00 × 00	0.00 × 00	*0.001	NS 0.556	ND	*<0.001
2-Octanone	111-13-7	1034	5.44×10^6	5.16×10^6	3.37×10^6	1.27×10^7	1.89×10^7	3.45×10^7	2.69×10^7	1.87×10^7	1.43×10^7	NS 0.071	NS 0.330	NS 0.226	*0.011
2-Pentanone	107-87-9	727	7.97×10^7	6.78×10^7	6.73×10^7	1.06×10^8	5.82×10^7	7.97×10^8	1.40×10^8	6.48×10^7	6.08×10^7	*<0.001	NS 0.726	NS 0.235	*<0.001
2-Undecanone	112-12-9	1353	0.00 × 00	0.00 × 00	0.00 × 00	8.09×10^6	0.00 × 00	1.50×10^8	1.86×10^7	0.00 × 00	0.00 × 00	*0.001	NS 0.516	ND	*<0.001
3-Hexen-2-one	763-93-9	839	1.20×10^7	1.70×10^6	0.00 × 00	5.93×10^6	9.68×10^6	1.05×10^7	3.80×10^6	0.00 × 00	0.00 × 00	NS 0.065	NS 0.244	NS 0.129	NS 0.111
3,5-(<i>E,E</i>)-Octadien-2-one (or isomer)	30086-02-3	1130	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	1.39×10^7	0.00 × 00	2.86×10^7	*<0.001	*0.002	ND	* 0.001
4-Methyl-3-pentene-2-one (tentative)	141-79-7	839	0.00 × 00	0.00 × 00	0.00 × 00	1.03×10^7	1.37×10^7	9.34×10^6	1.65×10^7	1.79×10^7	0.00 × 00	*0.001	*0.025	*<0.001	NS 0.211
4,6-Dimethyl-2-heptanone	19549-80-5	-	7.33×10^6	9.45×10^6	8.92×10^6	4.66×10^6	3.16×10^6	0.00 × 00	9.63×10^6	1.22×10^7	1.91×10^7	NS 0.187	NS 0.766	NS 0.071	NS 0.117
5-Hepten-2-one (tentative)	6714-00-7	921	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	7.28×10^7	0.00 × 00	0.00 × 00	0.00 × 00	*<0.001	ND	NS	*<0.001
Acetone	67-64-1	532	1.23×10^9	9.62×10^8	1.20×10^9	1.24×10^9	5.67×10^8	7.51×10^8	1.15×10^9	6.00×10^8	1.20×10^9	*0.041	NS 0.959	NS 0.218	*<0.001
Acetophenone	98-86-2	1030	3.90×10^6	2.18×10^6	3.56×10^6	4.80×10^6	0.00 × 00	2.70×10^6	1.57×10^6	5.82×10^5	8.14×10^5	*0.048	NS 0.260	NS 0.170	NS 0.224
Cyclohexanone	108-94-1	956	8.34×10^5	8.05×10^6	5.36×10^6	1.74×10^6	9.14×10^5	0.00 × 00	0.00 × 00	1.93×10^6	0.00 × 00	NS 0.338	NS 0.574	NS 0.054	NS 0.117
Acetyl valeryl (2,3-heptanedione)	96-04-8	875	3.25×10^6	1.46×10^6	3.68×10^6	5.53×10^6	2.14×10^6	7.10×10^6	2.38×10^6	6.73×10^6	1.80×10^6	NS 0.680	NS 0.701	NS 0.364	NS 0.347

Table 1. Chemicals and their associated hazard values															
Chemical	EC No.	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)	LD50 (mg/kg)
Methyl Isobutyl Ketone	108-10-1	780	3.08×10^8	1.84×10^8	2.41×10^8	3.12×10^8	1.67×10^8	1.80×10^8	3.25×10^8	1.70×10^8	2.45×10^8	*0.045	NS 0.982	0.512	*0.027
Ester															
Ethyl heptanoate	106-30-9	1120	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	3.77×10^6	8.69×10^6	0.00×00	0.00×00	NS 0.421	NS 0.422	ND	*<0.001
Ethyl (Z)-2-butenoate	6776-19-8	875	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	3.01×10^7	1.16×10^8	0.00×00	0.00×00	NS 0.468	NS 0.422	ND	*<0.001
Ethyl acetate	141-78-6	639	0.00×00	0.00×00	0.00×00	7.91×10^6	0.00×00	6.48×10^7	9.66×10^7	0.00×00	0.00×00	NS 0.334	NS 0.449	ND	*<0.001
Ethyl decanoate	110-38-3	1419	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	2.24×10^8	0.00×00	0.00×00	NS 0.051	NS 0.163	ND	ND
Ethyl hexanoate	123-66-0	1021	0.00×00	0.00×00	0.00×00	1.34×10^8	0.00×00	3.79×10^9	2.37×10^9	0.00×00	0.00×00	0.021	NS 0.436	ND	*<0.001
Ethyl octanoate	106-32-1	1220	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	3.01×10^7	2.65×10^8	0.00×00	0.00×00	NS 0.445	NS 0.405	ND	*0.002
Ethyl pentanoate	539-82-2	923	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	3.07×10^7	2.13×10^7	0.00×00	0.00×00	*0.045	NS 0.422	ND	*<0.001
Ethyl propanoate	105-37-3	735	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	1.65×10^7	5.24×10^6	0.00×00	0.00×00	*0.039	NS 0.422	ND	NS 0.095
Methyl butanoate	105-54-4	747	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	2.16×10^7	0.00×00	0.00×00	0.00×00	*<0.001	ND	ND	*<0.001
Methyl hexanoate	123-66-0	949	0.00×00	0.00×00	0.00×00	6.18×10^5	0.00×00	2.74×10^7	6.60×10^5	0.00×00	0.00×00	*<0.001	NS 0.629	ND	*0.004
Methyl methacrylate	80-62-6	736	5.44×10^6	9.65×10^6	6.33×10^6	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	*0.007	NS 0.087	NS 0.079	*<0.001
Alcohol															
2-Methyl-1-butanol	137-32-6	715	5.50×10^7	8.54×10^7	8.58×10^7	5.30×10^7	5.28×10^7	1.09×10^8	4.92×10^7	4.69×10^7	3.56×10^7	*<0.001	NS 0.851	*0.002	*0.003
3-Methyl-1-butanol	123-51-3	765	7.22×10^7	1.92×10^7	2.30×10^8	2.13×10^8	1.22×10^8	3.05×10^8	7.19×10^8	1.32×10^8	1.81×10^8	NS 0.321	NS 0.356	NS 0.323	NS 0.404

3-Dimethyl-2-butanol (tentative)	594-60-5	773	2.46×10^6	2.61×10^6	0.00×00	0.00×00	0.00×00	0.00×00	4.55×10^6	2.19×10^6	2.83×10^6	NS 0.054	NS 0.118	NS 0.959	*<0.001
Ethanol	64-17-5	505	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	7.39×10^7	7.00×10^8	0.00×00	0.00×00	NS 0.481	NS 0.422	NS	NS 0.082
1-Hexanol	111-27-3	894	1.63×10^6	7.06×10^5	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	*0.001	*<0.001	NS 0.422	ND
2-Ethyl-1-hexanol	104-76-7	1075	4.60×10^7	5.01×10^7	3.65×10^7	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	*<0.001	*<0.001	*0.001	*<0.001
1-Octanol	111-87-5	1116	0.00×00	0.00×00	2.56×10^6	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	2.20×10^7	*<0.001	ND	ND	*<0.001
1-Pentanol	71-41-0	794	1.11×10^9	1.20×10^9	1.01×10^8	6.45×10^8	7.05×10^8	3.48×10^7	4.18×10^8	3.05×10^8	4.67×10^7	*<0.001	*<0.001	*<0.001	*0.040
Isopropyl Alcohol	67-63-0	451	0.00×00	0.00×00	0.00×00	3.31×10^6	0.00×00	3.93×10^7	2.58×10^7	0.00×00	0.00×00	NS 0.147	*<0.001	ND	NS 0.083
Acid															
Propanoic acid, 2-methyl-, 3-hydroxy-2,2,4-trimethylpentyl ester	77-68-9	1460	3.82×10^7	1.38×10^7	0.00×00	6.86×10^6	5.48×10^6	0.00×00	3.74×10^6	2.31×10^6	0.00×00	*0.023	NS 0.121	NS 0.340	ND
Terpene															
3-Carene	13466-78-9	1035	0.00×00	0.00×00	0.00×00	5.14×10^6	0.00×00	0.00×00	0.00×00	0.00×00	0.00×00	NS 0.192	NS 0.276	NS	ND
α -Pinene	80-56-8	953	1.01×10^7	8.21×10^6	3.97×10^6	8.04×10^7	2.80×10^7	3.25×10^7	1.56×10^7	7.54×10^6	3.19×10^6	*<0.001	*0.023	*0.004	*0.020
Cumene	98-82-8	990	5.37×10^5	2.26×10^6	1.07×10^6	3.59×10^6	2.03×10^5	9.07×10^6	5.11×10^6	3.59×10^6	1.31×10^6	*<0.001	NS 0.093	NS 0.130	*0.002
D-Limonene	5989-27-5	1055	2.15×10^7	1.34×10^7	1.08×10^7	6.08×10^6	2.63×10^6	0.00×00	0.00×00	0.00×00	0.00×00	*0.001	*0.003	NS 0.148	*0.001
Mesitylene	108-67-8	1028	8.50×10^7	5.33×10^7	5.03×10^7	5.68×10^7	2.55×10^7	5.06×10^7	5.13×10^7	3.32×10^7	3.18×10^7	NS 0.151	NS 0.522	*0.025	NS 0.172

trans-β-Ocimene (or isomer)	3779-61-1	1035	0.00 × 00	0.00 × 00	1.08 × 10 ⁷	4.38 × 10 ⁶	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	*0.002	NS 0.422	ND	*0.001
Furan															
2,4-Dimethylfuran	3710-43-8	732	1.38 × 10 ⁷	1.26 × 10 ⁷	6.20 × 10 ⁶	1.27 × 10 ⁷	4.19 × 10 ⁶	9.01 × 10 ⁶	9.23 × 10 ⁶	1.22 × 10 ⁷	1.54 × 10 ⁶	NS 0.265	NS 0.820	NS 0.183	*0.020
2,5-Dimethylfuran	625-86-5	734	1.55 × 10 ⁷	1.03 × 10 ⁷	3.76 × 10 ⁶	1.42 × 10 ⁷	4.19 × 10 ⁶	9.01 × 10 ⁶	1.96 × 10 ⁸	1.17 × 10 ⁸	7.36 × 10 ⁷	NS 0.452	NS 0.648	NS 0.618	*0.049
2-Ethylfuran	3208-16-0	717	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	7.87 × 10 ⁶	1.12 × 10 ⁷	1.54 × 10 ⁶	NS 0.114	NS 0.326	NS 0.422	NS 0.124
Hydrocarbon															
2,4-Di-tert-butylphenol	96-76-4	1595	0.00 × 00	0.00 × 00	0.00 × 00	1.30 × 10 ⁷	1.81 × 10 ⁶	9.30 × 10 ⁶	3.94 × 10 ⁶	0.00 × 00	0.00 × 00	*0.021	NS 0.108	NS 0.422	NS 0.089
2,6-Bis(1,1-dimethylethyl)-4-(1-oxopropyl)phenol (tentative)	14035-34-8	1684	2.29 × 10 ⁷	1.12 × 10 ⁷	8.54 × 10 ⁶	2.82 × 10 ⁷	1.49 × 10 ⁷	2.18 × 10 ⁷	1.81 × 10 ⁷	2.89 × 10 ⁷	2.55 × 10 ⁷	NS 0.463	NS 0.801	*0.048	NS 0.163
2,4-Dimethylbenzaldehyde	15764-16-6	1305	3.50 × 10 ⁶	5.16 × 10 ⁶	3.50 × 10 ⁶	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	*0.001	*0.008	*0.025	*0.048
Benzene	71-43-2	684	7.00 × 10 ⁶	5.78 × 10 ⁶	4.10 × 10 ⁶	4.71 × 10 ⁶	2.68 × 10 ⁶	6.17 × 10 ⁶	2.55 × 10 ⁶	2.32 × 10 ⁶	4.06 × 10 ⁶	NS 0.542	NS 0.154	NS 0.331	NS 0.756
1,2,3-Trimethylbenzene	526-73-8	1028	8.50 × 10 ⁷	5.33 × 10 ⁷	5.03 × 10 ⁷	5.68 × 10 ⁷	2.55 × 10 ⁷	5.06 × 10 ⁷	5.13 × 10 ⁷	3.32 × 10 ⁷	3.18 × 10 ⁷	NS 0.151	NS 0.522	*0.025	NS 0.172
1,3-bis(1,1-dimethylethyl)-benzene	1014-60-4	1284	5.04 × 10 ⁸	6.01 × 10 ⁸	4.70 × 10 ⁸	4.46 × 10 ⁸	3.33 × 10 ⁸	5.35 × 10 ⁸	5.30 × 10 ⁸	4.51 × 10 ⁸	3.09 × 10 ⁸	NS 0.247	NS 0.902	*0.003	*<0.001
Ethylbenzene	100-41-4	897	9.72 × 10 ⁷	7.10 × 10 ⁷	5.62 × 10 ⁷	1.37 × 10 ⁸	6.50 × 10 ⁷	1.71 × 10 ⁸	1.96 × 10 ⁸	1.17 × 10 ⁸	7.36 × 10 ⁷	*0.032	NS 0.427	*0.003	*<0.001
o-Cymene	527-84-4	1055	1.22 × 10 ⁶	4.97 × 10 ⁵	0.00 × 00	3.10 × 10 ⁶	4.71 × 10 ⁵	1.25 × 10 ⁶	0.00 × 00	0.00 × 00	0.00 × 00	*0.016	*0.015	NS 0.629	NS 0.422
o-xylene	95-47-6	897	7.42 × 10 ⁷	5.95 × 10 ⁷	5.60 × 10 ⁷	8.02 × 10 ⁷	3.98 × 10 ⁷	1.08 × 10 ⁸	1.04 × 10 ⁸	5.92 × 10 ⁷	5.09 × 10 ⁷	NS 0.185	NS 0.768	*0.010	*0.010

<i>p</i> -Cresol	106-44-5	1182	0.00 × 00	0.00 × 00	0.00 × 00	3.58 × 10 ⁸	1.06 × 10 ⁸	1.51 × 10 ⁸	5.93 × 10 ⁷	2.03 × 10 ⁷	1.88 × 10 ⁷	*0.013	NS 0.116	*<0.001	*<0.001
<i>p</i> -Xylene	106-42-3	895	9.72 × 10 ⁷	7.10 × 10 ⁷	5.62 × 10 ⁷	1.37 × 10 ⁸	6.50 × 10 ⁷	1.71 × 10 ⁸	1.96 × 10 ⁸	1.17 × 10 ⁸	7.36 × 10 ⁷	*0.032	NS 0.427	* 0.003	*<0.001
Styrene	100-42-5	927	4.87 × 10 ⁶	4.63 × 10 ⁶	0.00 × 00	0.00 × 00	1.12 × 10 ⁷	0.00 × 00	7.15 × 10 ⁶	2.14 × 10 ⁶	5.53 × 10 ⁶	NS 0.105	NS 0.241	NS 0.233	NS 0.090
tert-Butylbenzene	98-06-6	1024	1.39 × 10 ⁷	1.71 × 10 ⁷	7.51 × 10 ⁶	1.17 × 10 ⁷	8.23 × 10 ⁶	1.33 × 10 ⁷	1.17 × 10 ⁷	1.29 × 10 ⁷	6.30 × 10 ⁶	NS 0.324	NS 0.889	NS 0.121	NS 0.287
Toluene	108-88-3	792	2.42 × 10 ⁹	1.30 × 10 ⁹	6.28 × 10 ⁷	2.41 × 10 ⁹	1.23 × 10 ⁹	4.91 × 10 ⁷	2.35 × 10 ⁹	1.15 × 10 ⁹	4.73 × 10 ⁷	*<0.001	NS 0.996	NS 0.281	*0.035
Phenolic															
Phenol	108-95-2	1093	0.00 × 00	0.00 × 00	0.00 × 00	7.60 × 10 ⁶	1.23 × 10 ⁶	0.00 × 00	4.96 × 10 ⁶	1.05 × 10 ⁶	7.23 × 10 ⁵	NS 0.074	NS 0.343	NS 0.626	NS 0.422
Sulfur															
Dimethyl sulfide	75-18-3	536	9.61 × 10 ⁶	5.73 × 10 ⁶	2.29 × 10 ⁶	1.40 × 10 ⁷	2.36 × 10 ⁶	2.89 × 10 ⁷	6.23 × 10 ⁷	1.16 × 10 ⁶	0.00 × 00	NS 0.402	NS 0.501	NS 0.409	*<0.001
Dimethyl sulfone	67-71-0	1052	1.77 × 10 ⁷	3.34 × 10 ⁶	0.00 × 00	2.60 × 10 ⁷	9.68 × 10 ⁶	0.00 × 00	1.11 × 10 ⁷	1.34 × 10 ⁶	0.00 × 00	*0.001	NS 0.277	NS 0.200	ND
Methanethiol	74-93-1	459	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	0.00 × 00	9.25 × 10 ⁶	0.00 × 00	0.00 × 00	0.00 × 00	*<0.001	ND	ND	*<0.001
Ether															
Ethyl ether	60-29-7	514	8.30 × 10 ⁶	1.01 × 10 ⁷	9.61 × 10 ⁶	7.75 × 10 ⁶	7.17 × 10 ⁶	2.51 × 10 ⁶	5.50 × 10 ⁶	4.57 × 10 ⁶	4.81 × 10 ⁶	NS 0.886	NS 0.865	NS 0.661	NS 0.399
Vinylisopentyl ether	39782-38-2	767	3.91 × 10 ⁷	2.04 × 10 ⁸	2.96 × 10 ⁸	1.84 × 10 ⁸	6.42 × 10 ⁷	1.97 × 10 ⁸	1.21 × 10 ⁸	6.23 × 10 ⁷	5.10 × 10 ⁷	NS 0.111	NS 0.126	NS 0.397	NS 0.094

Table S6. The 26 sensory descriptors applied to the three pasteurized milk samples (grass (GRS), clover (CLV) and total mixed ration (TMR)) by full descriptive sensory analysis.

Section	Descriptor
Aroma	
	1. Dairy sweet aroma
	2. Cooked milk
	3. Barnyard aroma
	4. Grassy aroma
	5. Hay like aroma
	6. Malty aroma
Flavor	
	7. Dairy sweet flavor
	8. Cooked milk flavor
	9. Dairy fat flavor
	10. Malty flavor
	11. Creamy flavor
	12. Hay like flavor
	13. Grassy flavor
	14. Dairy sour flavor
	15. Off flavor
Mouth feel	
	16. Viscosity
	17. Creaminess
	18. Mouth coating
	19. Chalkiness
After effect (AE)	
	20. Astringency
	21. Mouth coating AE
	22. Dairy sweet AE
	23. Cooked milk AE
	24. Dairy sour AE
	25. Malty AE

26. Barnyard AE
