

Supplementary Materials

An untargeted metabolomic comparison of milk composition from sheep kept under different grazing systems

Table S1. GC-MS metabolite characteristics.

Metabolite	RT(min) ^a	<i>m/z</i> ^b
Lactic acid	15.86	117,147,191
Glycolic acid	16.16	147,205,73
Unk ^c #1	17.08	258,116,147
Unk #2	17.45	147,133,220
Glycine	17.21	102,147,204
Ethanodioic acid	17.44	133,235,220
Phosphate	18.14	241,281,242
Urea	19.19	189,148,190
Ethanolamine	19.55	174,100,147
Phosphate	19.71	299,314,211
Succinic acid	20.19	75,148,247
Glyceric acid	20.54	292,147,189
Malic acid	22.64	233,147,245
Glutaric acid	23.70	75,198,156
Ribose	25.04	217,103,307
Xylitol	25.52	217,103,205
Glucitol	25.60	117,160,75
Fucose	25.62	117,73,147
Orotic acid	25.67	254,147,357
Galactopyranose	25.77	73,130,204
Phosphate	25.91	357,299,358
Citric acid	26.51	273,147,363
Hippuric acid	26.60	206,105,236
Erythrose	26.64	217,218,204
Asparagine	26.66	217,204,191
Glucopyranose	26.71	217,204,218
Fructose	27.17	103,217,307
Galactose	27.38	319,73,205
Hexose	27.40	319,205,147
Glucose	27.44	319,320,160
Glycerol	27.54	303,205,133
Hexose	27.62	319,205,147
Unk #3	27.86	217,218,246
Gluconic Acid	28.00	319,217,333
Altrose	28.11	319,217,129
Palmitic Acid	28.54	313,117,75

<i>Scyllo</i> -inositol	28.73	318,217,191
Galactofuranose	29.03	217,218,246
N-Acetylglucosamine	29.21	73,319,205
<i>Myo</i> -inositol	29.31	305,217,318
Glucose	29.56	319,205,320
Stearic acid	30.32	341,117,73
Uridine	32.26	217,169,217
Inosine	33.24	217,230,245
Lactose	34.40	204,361,217
Maltose	35.13	204,191,217

a) RT retention time (min); b) EI-MS, m/z (amu); c) not annotated metabolite.

Figure S1. PCA score plot in the first and third components (50 % of variance expressed) of GS2 (n= 33, empty circles) and GS1 (n= 37, empty boxes) milk samples, based on their GC-MS features.

