

An untargeted metabolomics investigation of Milk from Dairy Cows with Clinical Mastitis by ^1H -NMR

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Table S1 Information for molecules identification by means of ^1H -NMR

	Functional Group	Multiplicity	ppm
2-Hydroxyisobutyrate	CH_3	s	1.3466
2-Oxoglutarate	CH_2 -4	t	2.4279
3-Hydroxybutyrate	CH_3	d	1.1917
Acetate	CH_3	s	1.9071
Acetone	CH_3	s	2.2199
Alanine	CH_3	d	1.4756
Arginine	CH_2 -3	m	1.8964
Betaine	CH_3	s	3.2511
Carnitine	CH_3	s	3.2040
Choline	CH_3	s	3.1889
<i>cis</i> -Aconitate	CH_2	d	3.1107
Citrate	CH_2	d	2.5344
Creatine	CH_3	s	3.0231
Creatine phosphate	CH_3	s	3.0302
Creatinine	CH_3	s	3.0357
Cytidine	CH -6	d	6.1161
Dimethyl sulfone	CH_3	s	3.1418
Dimethylamine	CH_3	s	2.7100
Ethanol	CH_3	t	1.1692
Formate	CH	s	8.4437
Fumarate	CH	s	6.5087
Galactose	CH	d	5.2610
Glucose	CH	d	4.6320
Glucose-1-phosphate	CH	dd	5.4601
Glutamate	CH_2 -4	m	2.3363
Glycine	CH_2	s	3.5530
Hippurate	CH -3	t	7.5564
Histidine	CH	s	8.0919
Isobutyrate	CH_3	d	1.0615
Isoleucine	CH_3 -4	d	1.0007
Lactate	CH_3	d	1.3222

Lactose	CH-2	t	3.2869
Leucine	CH ₃	t	0.9464
Lysine	CH ₂ -6	t	3.0150
Malonate	CH ₂	s	3.1238
Maltose	CH	d	5.4001
N,N-Dimethylglycine	CH ₃	s	2.9039
N-Acetylglucosamine	CH ₃	s	2.0436
O-Acetylcarnitine	CH ₃	s	3.1781
Phenylalanine	CH-6	t	7.4142
Pimelate	CH ₂ -2	t	2.1449
Proline	CH ₂ -5	m	3.3509
Propionate	CH ₃	t	1.0540
Propylene glycol	CH ₃	d	1.1212
Pyruvate	CH ₃	s	2.3616
<i>sn</i> -Glycero-3-phosphocholine	CH ₃	s	3.2147
Succinate	CH ₂	s	2.3949
<i>trans</i> -Aconitate	CH-2	s	6.5782
Trimethylamine N-oxide	CH ₃	s	3.2593
Tyrosine	CH-6	d	6.9021
Uracil	CH-2	d	5.7917
Uridine	CH-4	t	5.9087
Valine	CH ₃	d	0.9770
Xylose	CH	d	4.5790

S stands for singlet, d stands for doublet, t stands for triplet and m stands for multiple signals.