

An untargeted metabolomics investigation of Jiulong Yak (*Bos grunniens*) meat by ¹H-NMR

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SUPPLEMENTAL MATERIAL

Table S1 Concentrations (mmol/g, median (IQR)) of molecules quantified by ¹H-NMR

	<i>Triceps brachii</i> (TB)	<i>Biceps femoris</i> (BF)	<i>Longissimus thoracis</i> (LT)	<i>p</i>	<i>Trapezius</i> (TP)	Fold change (LT/TP)
Amino acids, Peptides and analogues						
Alanine	4.76x10 ⁻³ (1.33x10 ⁻³) ^a	5.31x10 ⁻³ (4.77x10 ⁻⁴) ^a	3.14x10 ⁻³ (9.50x10 ⁻⁴) ^b	0.003	3.56x10 ⁻³ (2.59x10 ⁻⁵)	0.88
Anserine	1.27x10 ⁻³ (5.68x10 ⁻⁴) ^a	1.54x10 ⁻³ (6.66x10 ⁻⁴) ^a	1.94x10 ⁻³ (6.45x10 ⁻⁴) ^a	0.164	1.06x10 ⁻³ (3.62x10 ⁻⁶)	1.83
<i>beta</i> -Alanine	1.14x10 ⁻⁴ (1.21x10 ⁻⁴) ^a	1.50x10 ⁻⁴ (1.84x10 ⁻⁴) ^a	1.12x10 ⁻⁴ (8.98x10 ⁻⁵) ^a	0.968	1.26x10 ⁻⁴ (1.36x10 ⁻⁵)	0.89
Betaine	2.39x10 ⁻³ (3.90x10 ⁻⁴) ^a	2.15x10 ⁻³ (5.25x10 ⁻⁴) ^a	1.79x10 ⁻³ (1.00x10 ⁻³) ^a	0.301	2.57x10 ⁻³ (4.09x10 ⁻⁵)	0.70
Carnosine	1.23x10 ⁻² (1.65x10 ⁻³) ^b	1.60x10 ⁻² (8.17x10 ⁻³) ^b	2.09x10 ⁻² (1.84x10 ⁻³) ^a	0.017	1.45x10 ⁻² (2.97x10 ⁻⁴)	1.44
Creatine	3.89x10 ⁻² (2.29x10 ⁻³) ^a	3.68x10 ⁻² (5.63x10 ⁻³) ^a	4.11x10 ⁻² (8.27x10 ⁻⁴) ^a	0.389	3.78x10 ⁻² (2.20x10 ⁻⁴)	1.09
Creatinine	5.71x10 ⁻⁴ (7.74x10 ⁻⁵) ^a	4.95x10 ⁻⁴ (2.89x10 ⁻⁴) ^a	7.84x10 ⁻⁴ (8.11x10 ⁻⁵) ^a	0.094	6.22x10 ⁻⁴ (6.66x10 ⁻⁵)	1.26
Glutamate	1.06x10 ⁻³ (2.77x10 ⁻⁴) ^a	1.41x10 ⁻³ (5.55x10 ⁻⁴) ^a	7.68x10 ⁻⁴ (1.83x10 ⁻⁴) ^a	0.096	1.20x10 ⁻³ (9.25x10 ⁻⁵)	0.64
Glutamine	3.75x10 ⁻³ (3.15x10 ⁻³) ^a	3.26x10 ⁻³ (1.28x10 ⁻³) ^a	1.49x10 ⁻³ (1.63x10 ⁻⁴) ^a	0.051	3.87x10 ⁻³ (1.35x10 ⁻⁴)	0.33 [*]
Glutathione	2.47x10 ⁻⁴ (9.01x10 ⁻⁶) ^a	2.80x10 ⁻⁴ (1.84x10 ⁻⁴) ^a	1.50x10 ⁻⁴ (5.71x10 ⁻⁵) ^a	0.136	1.96x10 ⁻⁴ (3.48x10 ⁻⁵)	0.77
Glycine	2.26x10 ⁻³ (1.13x10 ⁻³) ^a	2.25x10 ⁻³ (4.31x10 ⁻⁴) ^a	2.10x10 ⁻³ (2.49x10 ⁻⁴) ^a	0.280	1.77x10 ⁻³ (2.11x10 ⁻⁵)	1.18
Isoleucine	1.81x10 ⁻⁴ (3.39x10 ⁻⁵) ^{ab}	2.33x10 ⁻⁴ (6.07x10 ⁻⁵) ^a	1.69x10 ⁻⁴ (4.61x10 ⁻⁵) ^b	0.012	2.27x10 ⁻⁴ (1.19x10 ⁻⁵)	0.74
Leucine	3.54x10 ⁻⁴ (7.22x10 ⁻⁵) ^{ab}	4.70x10 ⁻⁴ (9.67x10 ⁻⁵) ^a	3.06x10 ⁻⁴ (9.42x10 ⁻⁵) ^b	0.007	4.31x10 ⁻⁴ (1.60x10 ⁻⁵)	0.71
Methionine	1.69x10 ⁻³ (5.95x10 ⁻⁴) ^a	1.25x10 ⁻³ (1.39x10 ⁻³) ^a	1.68x10 ⁻³ (1.29x10 ⁻³) ^a	0.597	5.14x10 ⁻³ (6.09x10 ⁻⁴)	0.33 [*]
N,N-Dimethylglycine	1.13x10 ⁻⁴ (6.30x10 ⁻⁶) ^a	1.06x10 ⁻⁴ (1.06x10 ⁻⁵) ^a	1.17x10 ⁻⁴ (4.17x10 ⁻⁶) ^a	0.479	1.10x10 ⁻⁴ (1.54x10 ⁻⁶)	1.06
Phenylalanine	2.48x10 ⁻⁴ (7.34x10 ⁻⁵) ^{ab}	3.37x10 ⁻⁴ (7.77x10 ⁻⁵) ^a	2.39x10 ⁻⁴ (4.65x10 ⁻⁵) ^b	0.013	3.10x10 ⁻⁴ (1.43x10 ⁻⁵)	0.77
Proline	1.80x10 ⁻⁴ (3.42x10 ⁻⁵) ^a	1.68x10 ⁻⁴ (5.06x10 ⁻⁵) ^a	1.35x10 ⁻⁴ (4.95x10 ⁻⁵) ^a	0.074	2.06x10 ⁻⁴ (2.28x10 ⁻⁵)	0.66
Taurine	3.05x10 ⁻³ (3.50x10 ⁻⁴) ^a	2.96x10 ⁻³ (9.75x10 ⁻³) ^a	2.88x10 ⁻³ (3.22x10 ⁻³) ^a	0.178	1.42x10 ⁻³ (2.03x10 ⁻⁵)	2.03 [*]
Threonine	3.25x10 ⁻⁴ (1.88x10 ⁻⁴) ^a	4.27x10 ⁻⁴ (1.55x10 ⁻⁴) ^a	2.49x10 ⁻⁴ (4.85x10 ⁻⁵) ^b	0.008	3.78x10 ⁻⁴ (4.45x10 ⁻⁵)	0.66
Tyrosine	1.86x10 ⁻⁴ (2.99x10 ⁻⁵) ^{ab}	2.02x10 ⁻⁴ (5.03x10 ⁻⁵) ^a	1.60x10 ⁻⁴ (3.46x10 ⁻⁵) ^b	0.011	2.37x10 ⁻⁴ (1.13x10 ⁻⁵)	0.67
Valine	3.28x10 ⁻⁴ (4.58x10 ⁻⁵) ^{ab}	3.99x10 ⁻⁴ (7.97x10 ⁻⁵) ^a	3.03x10 ⁻⁴ (7.23x10 ⁻⁵) ^b	0.019	3.85x10 ⁻⁴ (9.49x10 ⁻⁶)	0.79
Carbohydrates and Derivates						
1,3-Dihydroxyacetone	2.06x10 ⁻⁵ (9.59x10 ⁻⁶) ^a	2.08x10 ⁻⁵ (3.54x10 ⁻⁶) ^a	1.64x10 ⁻⁵ (4.54x10 ⁻⁶) ^a	0.875	1.97x10 ⁻⁵ (2.59x10 ⁻⁶)	0.83
Glucose	5.89x10 ⁻³ (7.36x10 ⁻⁴) ^a	6.17x10 ⁻³ (1.08x10 ⁻³) ^a	6.06x10 ⁻³ (5.26x10 ⁻⁵) ^a	0.950	6.18x10 ⁻³ (4.29x10 ⁻⁴)	0.89
Glucose-1-phosphate	4.95x10 ⁻⁴ (2.01x10 ⁻⁴) ^a	4.52x10 ⁻⁴ (1.14x10 ⁻⁴) ^a	5.68x10 ⁻⁴ (1.63x10 ⁻⁴) ^a	0.908	2.88x10 ⁻⁴ (1.21x10 ⁻⁵)	1.97
Mannose	2.73x10 ⁻⁴ (4.26x10 ⁻⁵) ^{ab}	3.11x10 ⁻⁴ (9.82x10 ⁻⁵) ^a	2.35x10 ⁻⁴ (3.08x10 ⁻⁵) ^b	0.039	1.77x10 ⁻⁴ (3.60x10 ⁻⁵)	1.33
Organic acids and Derivates						
2-Oxovalerate	5.95x10 ⁻⁵ (5.19x10 ⁻⁵) ^a	7.42x10 ⁻⁵ (4.89x10 ⁻⁵) ^a	6.78x10 ⁻⁵ (4.85x10 ⁻⁵) ^a	0.618	8.13x10 ⁻⁵ (1.47x10 ⁻⁵)	0.83
4-Hydroxybutyrate	8.86x10 ⁻⁵ (9.80x10 ⁻⁵) ^a	1.09x10 ⁻⁴ (8.26x10 ⁻⁵) ^a	7.61x10 ⁻⁵ (5.59x10 ⁻⁵) ^a	0.390	5.96x10 ⁻⁵ (8.73x10 ⁻⁶)	1.28

Acetate	3.23x10 ⁻⁴ (6.11x10 ⁻⁵) ^a	5.45x10 ⁻⁴ (2.67x10 ⁻⁴) ^a	4.11x10 ⁻⁴ (2.39x10 ⁻⁴) ^a	0.180	6.08x10 ⁻⁴ (1.08x10 ⁻⁴)	0.68
Acetoacetate	3.51x10 ⁻⁵ (5.08x10 ⁻⁶) ^a	3.65x10 ⁻⁵ (7.37x10 ⁻⁶) ^a	1.90x10 ⁻⁵ (4.20x10 ⁻⁶) ^a	0.108	2.67x10 ⁻⁵ (3.90x10 ⁻⁶)	0.71
Citrate	2.11x10 ⁻⁴ (6.38x10 ⁻⁵) ^a	1.29x10 ⁻⁴ (9.36x10 ⁻⁵) ^a	1.05x10 ⁻⁴ (5.27x10 ⁻⁵) ^a	0.274	1.16x10 ⁻⁴ (1.53x10 ⁻⁵)	0.90
Formate	7.43x10 ⁻⁵ (7.88x10 ⁻⁶) ^{ab}	6.94x10 ⁻⁵ (1.85x10 ⁻⁵) ^b	8.34x10 ⁻⁵ (5.95x10 ⁻⁶) ^a	0.012	1.01x10 ⁻⁴ (1.76x10 ⁻⁵)	0.82
Fumarate	1.75x10 ⁻⁴ (5.45x10 ⁻⁵) ^a	1.58x10 ⁻⁴ (3.61x10 ⁻⁵) ^a	1.07x10 ⁻⁴ (2.55x10 ⁻⁵) ^a	0.235	1.68x10 ⁻⁴ (3.49x10 ⁻⁶)	0.64
Lactate	9.91x10 ⁻² (1.18x10 ⁻²) ^a	9.79x10 ⁻² (1.60x10 ⁻²) ^a	1.03x10 ⁻¹ (9.46x10 ⁻³) ^a	0.464	9.82x10 ⁻² (1.04x10 ⁻³)	1.05
Malate	1.21x10 ⁻³ (4.08x10 ⁻⁴) ^a	1.36x10 ⁻³ (2.85x10 ⁻⁴) ^a	1.06x10 ⁻³ (1.02x10 ⁻⁴) ^a	0.147	1.28x10 ⁻³ (5.29x10 ⁻⁵)	0.83
Malonate	1.18x10 ⁻³ (6.98x10 ⁻⁵) ^a	1.24x10 ⁻³ (3.85x10 ⁻⁴) ^a	8.21x10 ⁻⁴ (3.50x10 ⁻⁴) ^a	0.258	9.72x10 ⁻⁴ (3.80x10 ⁻⁵)	0.84
Pyruvate	2.46x10 ⁻⁴ (1.71x10 ⁻⁴) ^a	1.40x10 ⁻⁴ (8.06x10 ⁻⁵) ^a	1.99x10 ⁻⁴ (1.61x10 ⁻⁴) ^a	0.656	1.17x10 ⁻⁴ (3.04x10 ⁻⁶)	1.70

Nucleosides, Nucleotides and Analogues

Hypoxanthine	5.01x10 ⁻³ (1.62x10 ⁻³) ^a	5.55x10 ⁻³ (1.10x10 ⁻³) ^a	4.24x10 ⁻³ (4.07x10 ⁻⁴) ^a	0.426	9.29x10 ⁻³ (1.63x10 ⁻⁴)	0.46 [*]
IMP	1.39x10 ⁻⁴ (1.74x10 ⁻⁴) ^{ab}	4.30x10 ⁻⁴ (2.29x10 ⁻⁴) ^a	1.20x10 ⁻⁴ (3.44x10 ⁻⁵) ^b	0.031	4.18x10 ⁻⁴ (3.91x10 ⁻⁵)	0.28 [*]
Inosine	1.73x10 ⁻⁴ (1.35x10 ⁻⁴) ^{ab}	3.81x10 ⁻⁴ (1.89x10 ⁻⁴) ^a	1.76x10 ⁻⁴ (4.33x10 ⁻⁵) ^b	0.021	3.97x10 ⁻⁴ (2.68x10 ⁻⁵)	0.44 [*]
myo-Inositol	1.46x10 ⁻³ (3.25x10 ⁻³) ^a	5.94x10 ⁻⁴ (2.56x10 ⁻³) ^a	1.71x10 ⁻⁴ (2.68x10 ⁻⁴) ^a	0.176	1.49x10 ⁻³ (1.02x10 ⁻⁴)	0.11 [*]
Niacinamide	4.77x10 ⁻⁴ (1.06x10 ⁻⁴) ^a	5.34x10 ⁻⁴ (1.20x10 ⁻⁴) ^a	5.79x10 ⁻⁴ (4.80x10 ⁻⁵) ^a	0.695	5.14x10 ⁻⁴ (6.78x10 ⁻⁶)	1.13
UMP	6.91x10 ⁻⁵ (1.81x10 ⁻⁵) ^a	7.74x10 ⁻⁵ (2.58x10 ⁻⁵) ^a	8.89x10 ⁻⁵ (2.03x10 ⁻⁵) ^a	0.511	4.89x10 ⁻⁵ (1.77x10 ⁻⁶)	1.82
Uridine	8.95x10 ⁻⁵ (2.35x10 ⁻⁵) ^a	8.84x10 ⁻⁵ (2.11x10 ⁻⁵) ^a	9.04x10 ⁻⁵ (7.09x10 ⁻⁶) ^a	0.794	1.36x10 ⁻⁴ (1.30x10 ⁻⁵)	0.66
Xanthine	2.82x10 ⁻⁴ (6.33x10 ⁻⁵) ^a	2.55x10 ⁻⁴ (4.63x10 ⁻⁵) ^a	3.09x10 ⁻⁴ (2.66x10 ⁻⁵) ^a	0.240	2.87x10 ⁻⁴ (1.60x10 ⁻⁵)	1.08

Miscellaneous

Acetoin	1.16x10 ⁻⁵ (1.50x10 ⁻⁶) ^a	1.12x10 ⁻⁵ (3.68x10 ⁻⁵) ^a	1.52x10 ⁻⁵ (6.62x10 ⁻⁵) ^a	0.428	4.46x10 ⁻⁶ (1.63x10 ⁻⁶)	3.42 [*]
Carnitine	8.77x10 ⁻³ (2.79x10 ⁻³) ^a	6.36x10 ⁻³ (8.25x10 ⁻⁴) ^a	5.30x10 ⁻³ (1.41x10 ⁻³) ^a	0.127	7.21x10 ⁻³ (6.45x10 ⁻⁴)	0.73
Choline	9.71x10 ⁻⁴ (6.22x10 ⁻⁴) ^a	5.44x10 ⁻⁴ (7.76x10 ⁻⁴) ^a	1.02x10 ⁻³ (7.20x10 ⁻⁴) ^a	0.727	3.44x10 ⁻³ (4.36x10 ⁻⁴)	0.30 [*]
Dimethyl sulfone	1.08x10 ⁻⁴ (5.30x10 ⁻⁶) ^a	9.97x10 ⁻⁵ (1.60x10 ⁻⁵) ^a	1.15x10 ⁻⁴ (6.61x10 ⁻⁶) ^a	0.597	1.03x10 ⁻⁴ (1.59x10 ⁻⁶)	1.12
Guanidoacetate	1.79x10 ⁻³ (7.67x10 ⁻⁴) ^a	2.27x10 ⁻³ (8.18x10 ⁻⁴) ^a	2.53x10 ⁻³ (5.43x10 ⁻⁴) ^a	0.107	1.40x10 ⁻³ (2.68x10 ⁻⁵)	1.80
Glycerol	4.96x10 ⁻³ (1.40x10 ⁻³) ^a	6.39x10 ⁻³ (1.32x10 ⁻³) ^a	5.63x10 ⁻³ (1.36x10 ⁻³) ^a	0.101	3.97x10 ⁻³ (1.62x10 ⁻⁴)	1.42
Methanol	3.25x10 ⁻⁴ (6.03x10 ⁻⁴) ^a	1.42x10 ⁻⁴ (3.73x10 ⁻⁴) ^a	7.63x10 ⁻⁵ (3.93x10 ⁻⁵) ^a	0.114	1.71x10 ⁻⁴ (5.24x10 ⁻⁶)	0.45 [*]
O-Acetylcarnitine	6.25x10 ⁻⁴ (3.56x10 ⁻⁴) ^a	3.60x10 ⁻⁴ (4.78x10 ⁻⁴) ^a	7.23x10 ⁻⁴ (3.97x10 ⁻⁴) ^a	0.841	2.18x10 ⁻³ (2.89x10 ⁻⁴)	0.33 [*]
Trimethylamine	2.32x10 ⁻⁵ (2.38x10 ⁻⁶) ^a	2.03x10 ⁻⁵ (4.49x10 ⁻⁶) ^a	1.49x10 ⁻⁵ (4.71x10 ⁻⁶) ^a	0.190	2.13x10 ⁻⁵ (8.27x10 ⁻⁷)	0.70

¹ Means with different letters (a, b and ab) are significantly different at p<0.05. * Molecules characterized by a the fold change below 0.5 or above 2 [32].

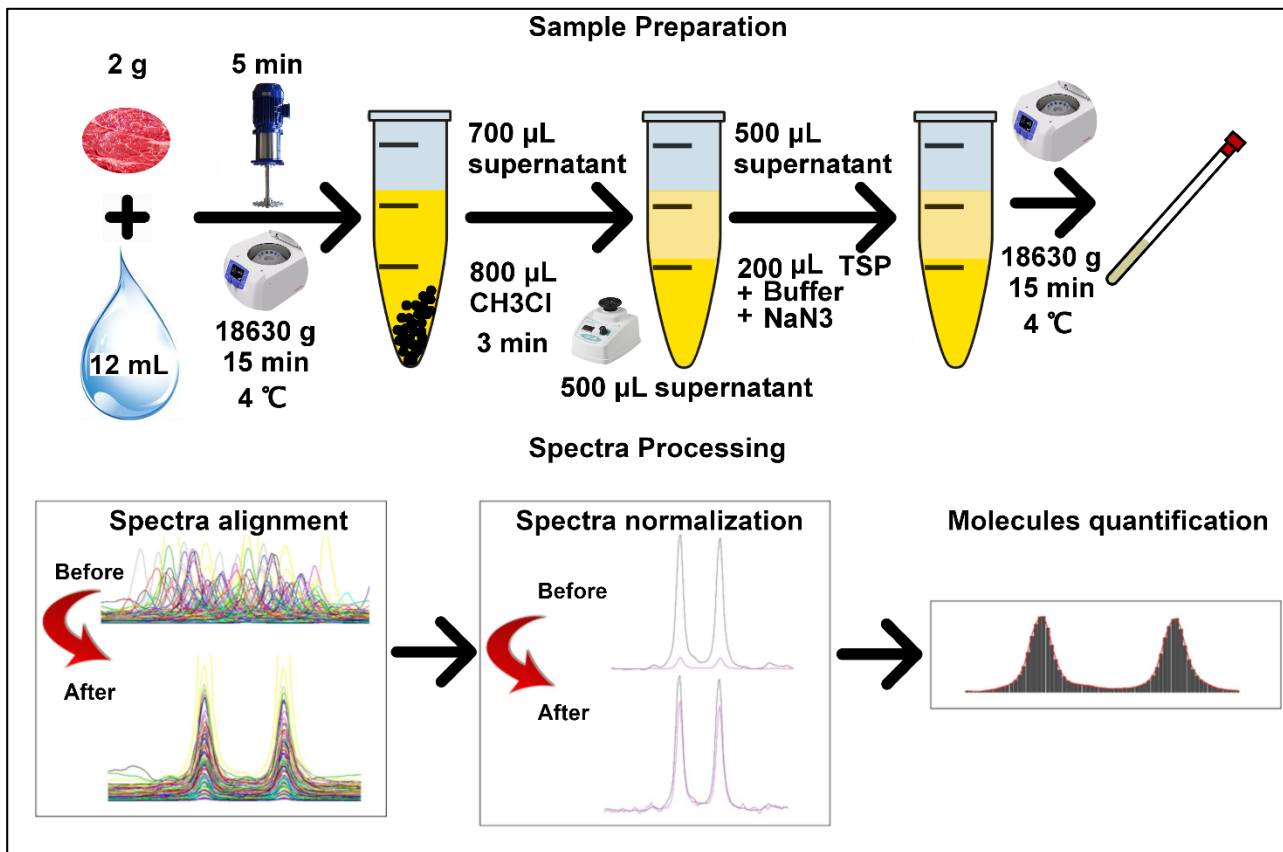
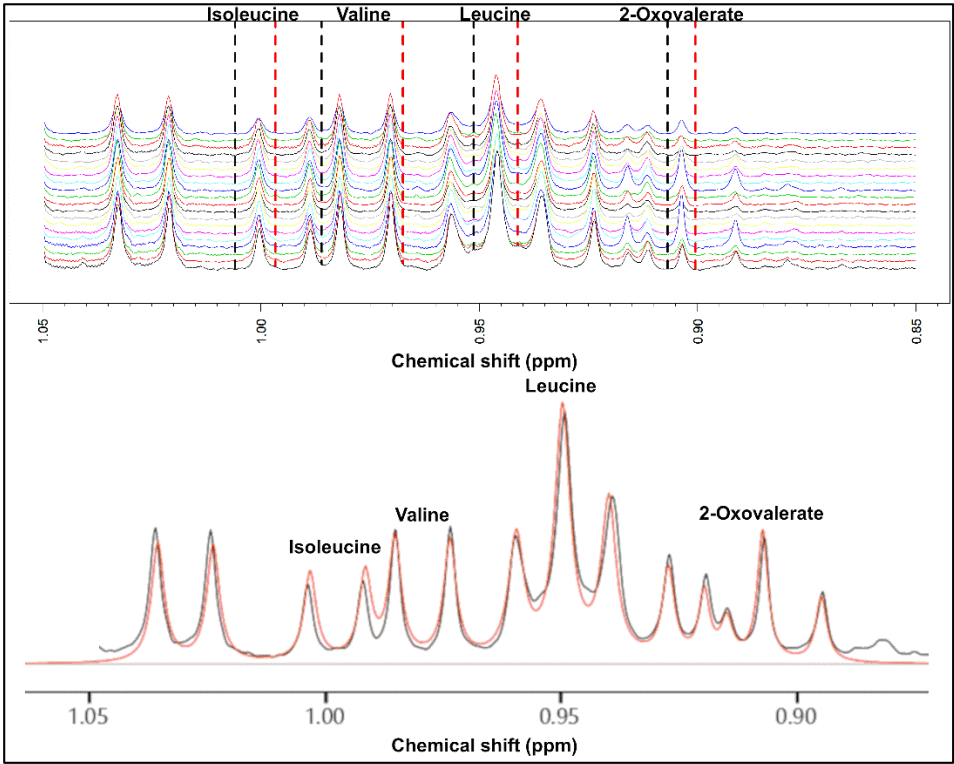


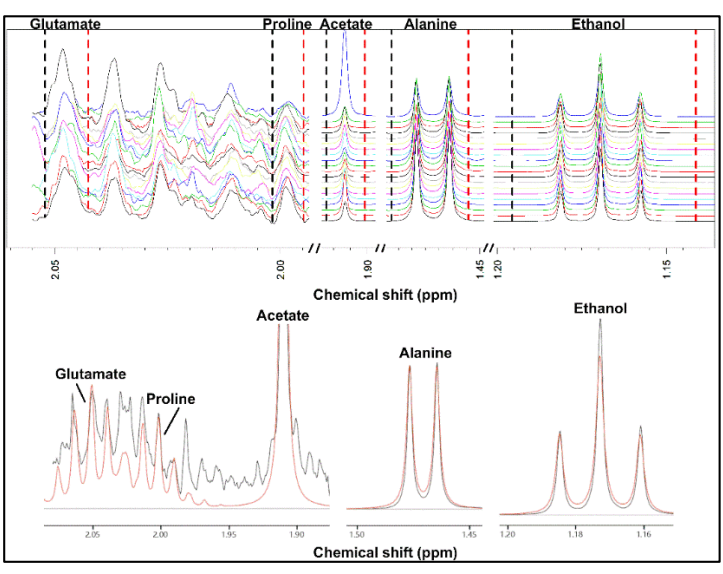
Figure S1. Graphic design of the workflow for meat samples preparation and ^1H -NMR spectra processing.

Figures S2-S13: Above panel - portions of the spectra, superimposed in white-washed mode. The black and red dashed lines show the portions of the spectra employed for the quantification of each molecule. Below – one representative spectrum (black line) superimposed to the signals simulated by software Chenomx (red line) for each of the molecules listed.

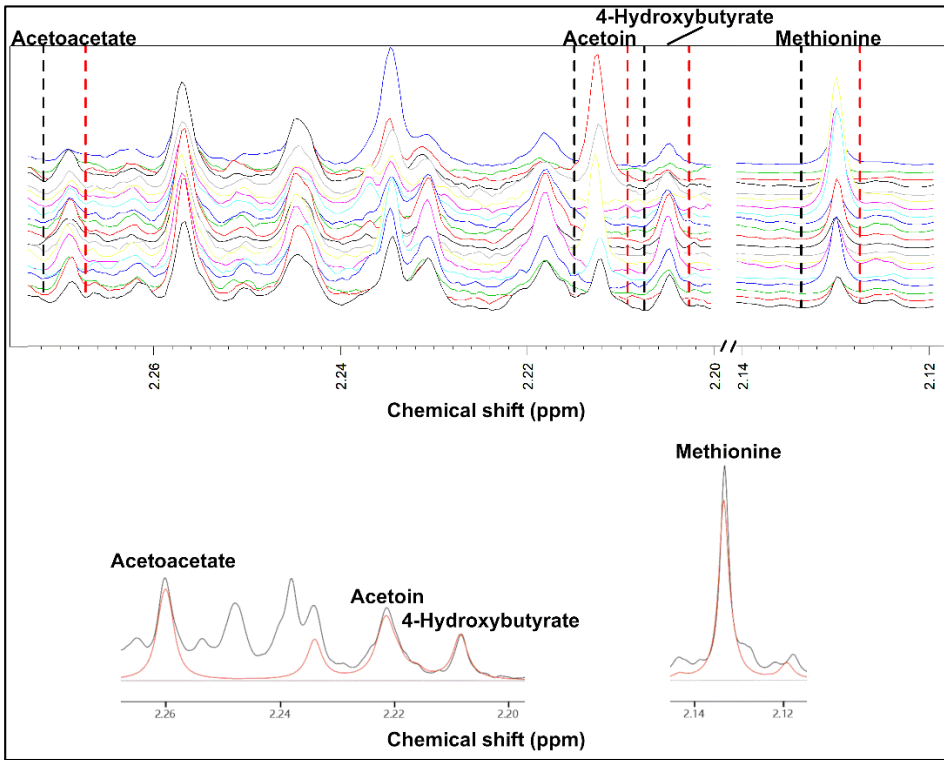
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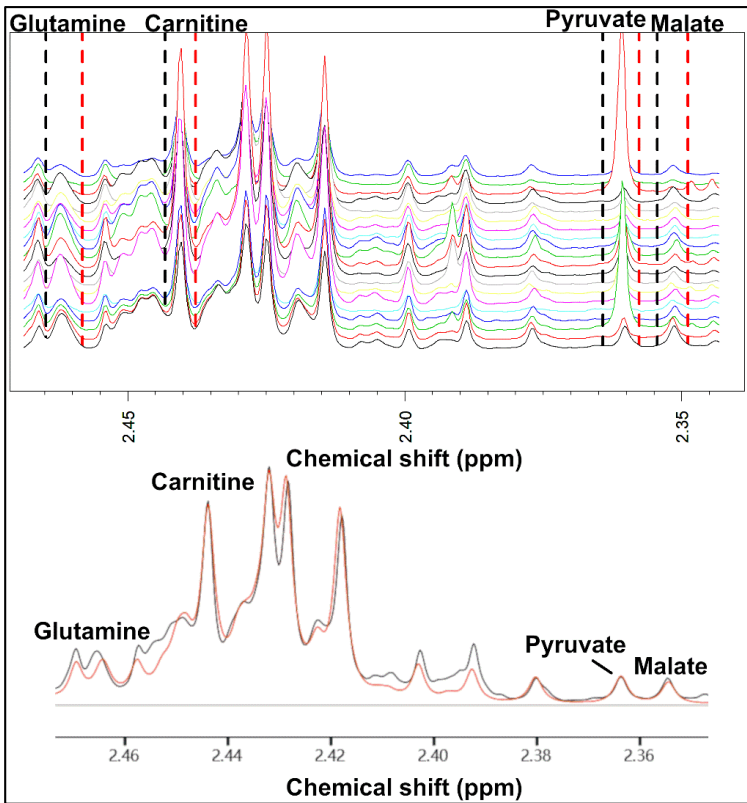
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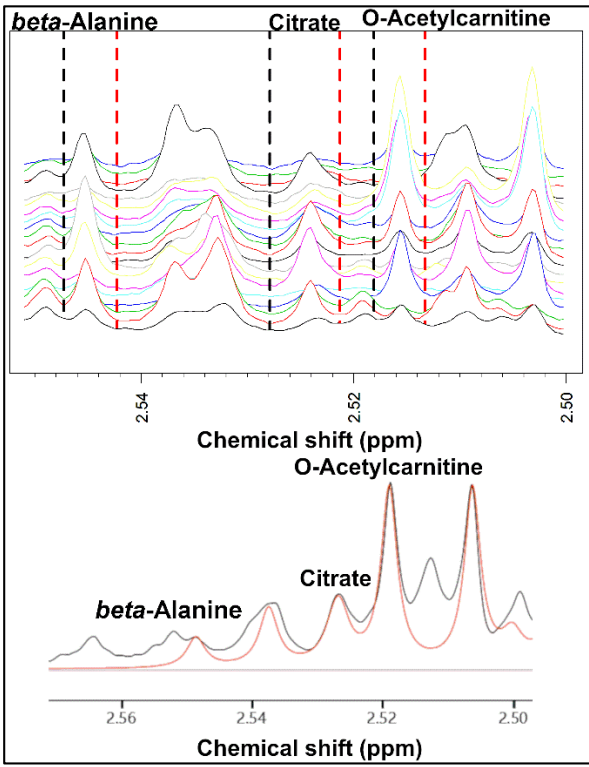
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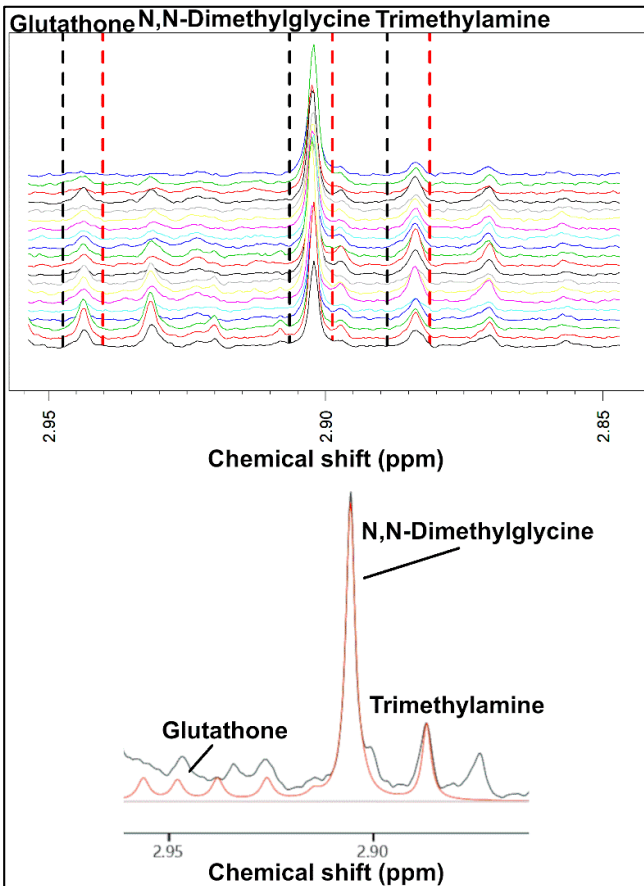
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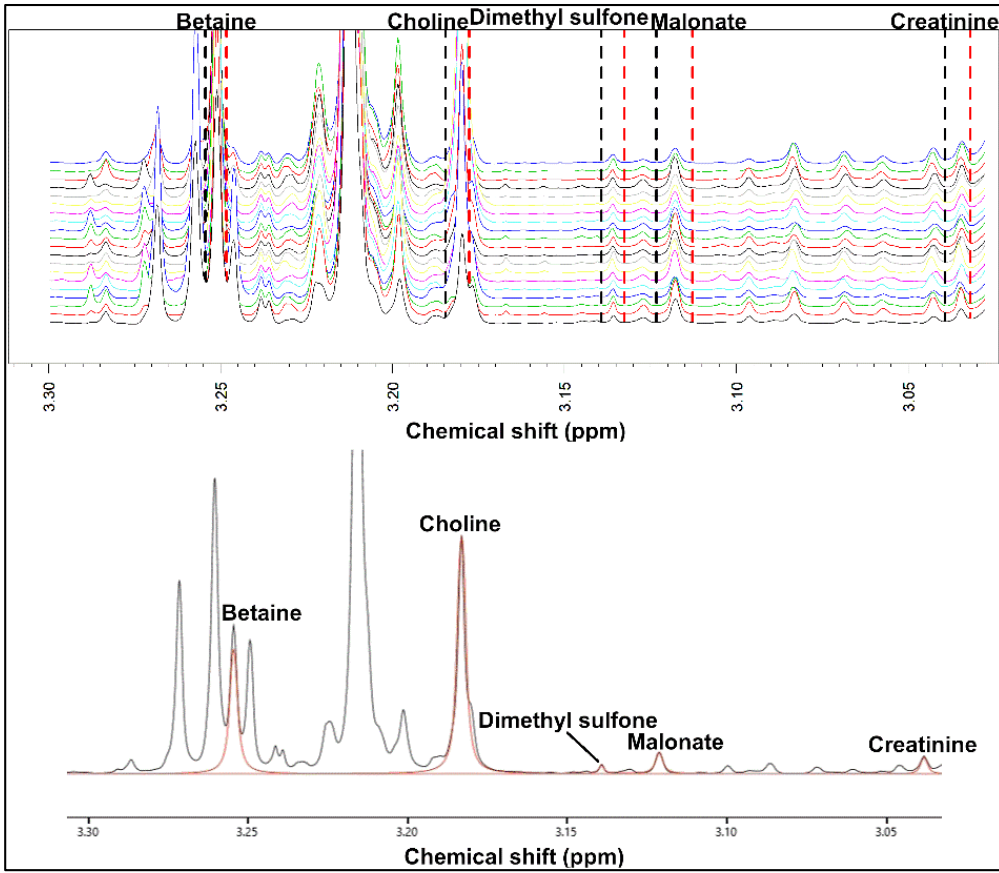
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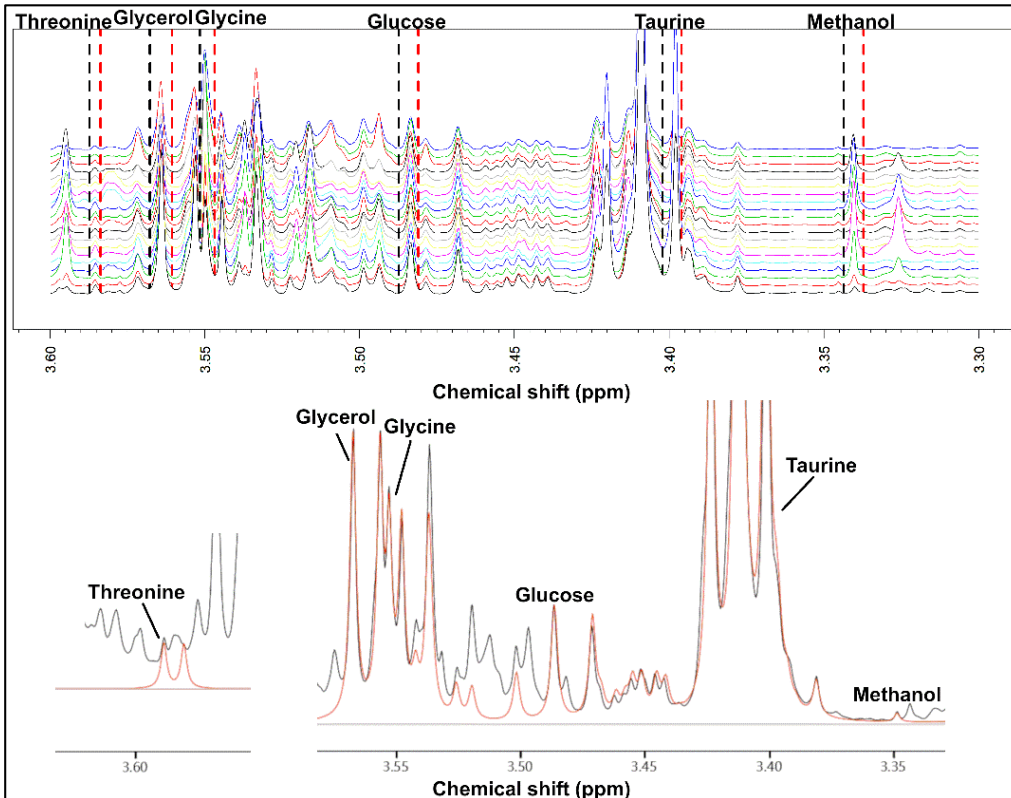
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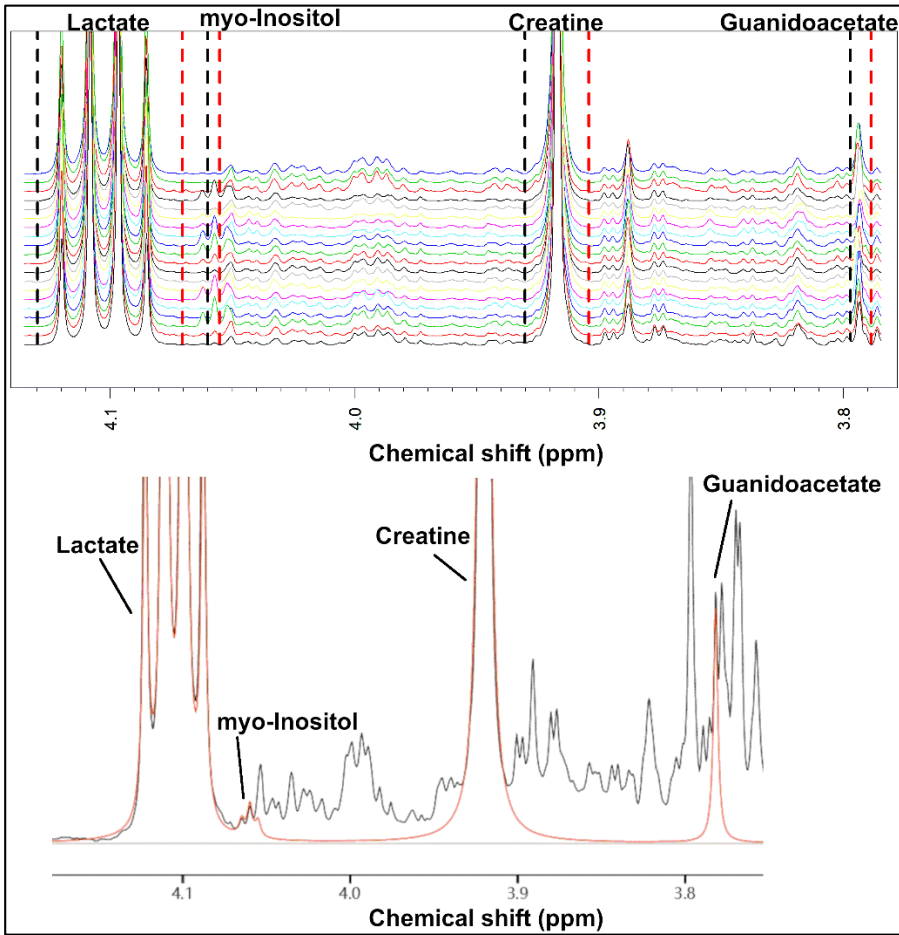
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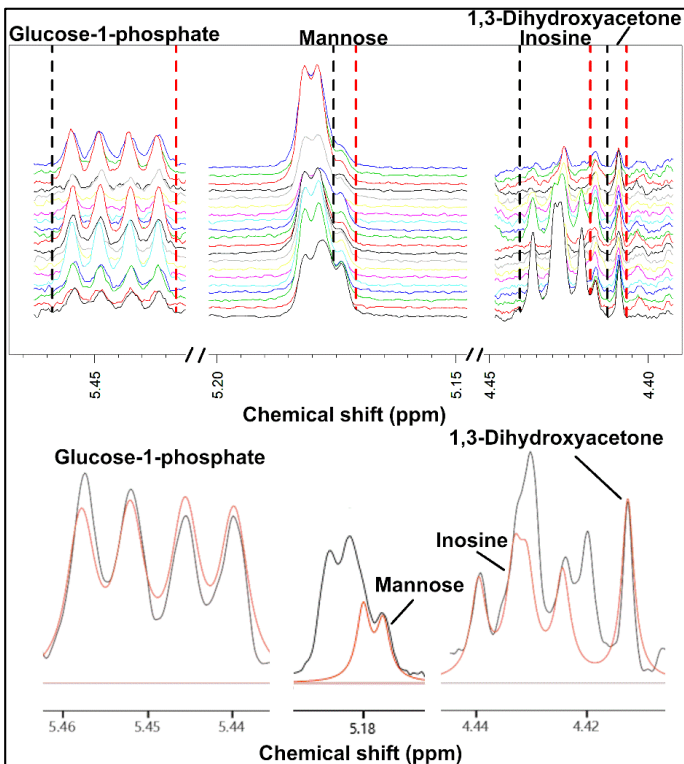
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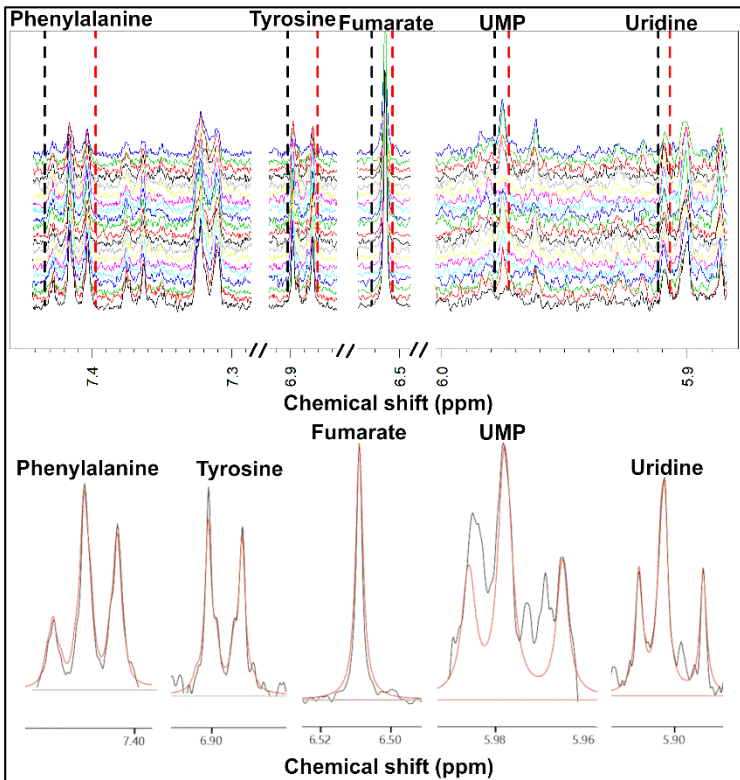
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