First insights into the urinary metabolome of captive giraffe by proton nuclear magnetic resonance spectroscopy

Chenglin Zhu[1#], Sabrina Fasoli[2#], Glori Isani[2], Luca Laghi[1*]

[1]Department of Agro-Food Science and Technology, University of Bologna, 47521, Cesena, Italy

[2]Department of Veterinary Medical Sciences, University of Bologna, Ozzano Emilia, 40064 Bologna, Italy

Table S1. Concentration (mmol/L, median (IQR)) of the molecules quantified by ^{1}H-NMR in all the samples studied in the present investigation, sorted by abundance.

Molecule	Concentration
Creatinine	20.9 (2.00)
Hippurate	19.1 (5.81)
Phenylacetylglycine	8.95 (2.13)
Allantoin	6.87 (2.46)
Benzoate	2.13 (7.38×10^{-1})
Acetate	1.49 (7.27×10^{-1})
Glycine	1.15 (6.96×10^{-1})
Glucuronate	8.68×10^{-1} (2.10×10^{-1})
Trimethylamine N-oxide	7.90×10^{-1} (6.22×10^{-1})
Dimethyl sulfone	7.40×10^{-1} (3.11×10^{-1})
Guanidoacetate	7.24×10^{-1} (1.59×10^{-1})
4-Hydroxyphenylacetate	5.84×10^{-1} (2.89×10^{-1})
Dimethylamine	5.14×10^{-1} (3.10×10^{-1})
N6-Acetyllysine	4.95×10^{-1} (1.20×10^{-1})
3-Methylglutarate	4.24×10^{-1} (1.08×10^{-1})
Formate	4.00×10^{-1} (1.56×10^{-1})
N-Isovaleroylglycine	2.90×10^{-1} (5.40×10^{-2})
cis-Aconitate	2.77×10^{-1} (5.18×10^{-2})
Pyroglutamate	2.62×10^{-1} (8.77×10^{-2})
Propionate	2.58×10^{-1} (1.38×10^{-1})
Taurine	2.02×10^{-1} (1.93×10^{-1})
Thymine	1.81×10^{-1} (7.96×10^{-2})
Lactate	1.75×10^{-1} (1.16×10^{-1})
Valerate	1.66×10^{-1} (6.32×10^{-2})
Betaine	1.64×10^{-1} (3.87×10^{-2})
3-Hydroxyisobutyrate	1.50×10^{-1} (1.93×10^{-2})

Succinate	$1.49x10^{-1}$ ($7.69x10^{-2}$)
Creatine	$1.45x10^{-1}$ ($3.64x10^{-2}$)
Ethanol	$1.17x10^{-1}$ ($4.65x10^{-2}$)
2-Oxovalerate	$1.14x10^{-1}$ ($2.84x10^{-2}$)
Sarcosine	$1.08x10^{-1}$ ($4.99x10^{-2}$)
2,6-Dihydroxybenzoate	$1.02x10^{-1}$ ($2.65x10^{-2}$)
Alanine	$8.55x10^{-2}$ ($2.68x10^{-2}$)
Citrate	$6.56x10^{-2}$ ($2.14x10^{-2}$)
N,N-Dimethylglycine	$6.27x10^{-2}$ ($6.07x10^{-2}$)
2-Hydroxyisobutyrate	$5.81x10^{-2}$ ($4.12x10^{-2}$)
Uracil	$5.55x10^{-2}$ ($1.83x10^{-2}$)
p-Cresol sulfate	$4.86x10^{-2}$ ($4.10x10^{-2}$)
Methylsuccinate	$2.43x10^{-2}$ ($7.11x10^{-3}$)

Table S2. Concentration (mmol/L) of the molecules quantified by ^{1}H-NMR in the samples collected during and after pregnancy.

	Giulietta		Nicole	
	Not Pregnant	**Pregnant**	**Not Pregnant**	**Pregnant**
Formate	$2.91x10^{-1}$	$3.03x10^{-1}$	$2.00x10^{-1}$	$2.82x10^{-1}$
Benzoate	2.14	3.88	2.46	12.22
2,6-Dihydroxybenzoate	$9.83x10^{-2}$	$1.82x10^{-1}$	$1.10x10^{-1}$	$1.07x10^{-1}$
Uracil	$6.27x10^{-2}$	$8.18x10^{-2}$	$8.60x10^{-2}$	$5.76x10^{-2}$
cis-Aconitate	$2.72x10^{-1}$	$2.55x10^{-1}$	$2.19x10^{-1}$	$2.09x10^{-1}$
Allantoin	6.76	9.86	9.87	6.53
Glucuronate	$7.18x10^{-1}$	$4.70x10^{-1}$	$3.70x10^{-1}$	$3.64x10^{-1}$
Hippurate	24.7	21.6	23.00	8.11
Betaine	$2.01x10^{-1}$	$1.46x10^{-1}$	$1.29x10^{-1}$	$1.24x10^{-1}$
Guanidoacetate	$8.07x10^{-1}$	$7.54x10^{-1}$	$4.95x10^{-1}$	$7.05x10^{-1}$
Phenylacetylglycine	10.20	3.52	10.40	5.02
Glycine	1.06	3.04	1.79	11.65
Acetoacetate	$4.27x10^{-2}$	$3.70x10^{-2}$	$4.33x10^{-3}$	$8.08x10^{-3}$
4-Hydroxyphenylacetate	$3.55x10^{-1}$	$3.62x10^{-1}$	$6.19x10^{-1}$	$7.81x10^{-1}$
Taurine	$1.75x10^{-1}$	$2.93x10^{-1}$	$7.98x10^{-2}$	$1.33x10^{-1}$
Trimethylamine N-oxide	1.36	1.38	1.52	1.44
Dimethyl sulfone	$9.76x10^{-1}$	1.09	$4.64x10^{-1}$	1.17
Creatinine	13.1	15.80	12.90	14.10
Creatine	$1.17x10^{-1}$	$9.12x10^{-2}$	$1.27x10^{-1}$	$1.22x10^{-1}$
N,N-Dimethylglycine	$6.22x10^{-2}$	$9.52x10^{-2}$	$2.49x10^{-2}$	$1.28x10^{-1}$
Sarcosine	$1.74x10^{-1}$	$1.66x10^{-1}$	$1.12x10^{-1}$	$2.01x10^{-1}$
Dimethylamine	$5.16x10^{-1}$	$9.48x10^{-1}$	$8.00x10^{-1}$	$9.72x10^{-1}$
Citrate	$3.14x10^{-2}$	$2.70x10^{-2}$	$3.82x10^{-2}$	$4.07x10^{-2}$
Succinate	$1.32x10^{-1}$	$5.26x10^{-2}$	$1.98x10^{-1}$	$1.56x10^{-1}$

Pyroglutamate	$3.28x10^{-1}$	$3.24x10^{-1}$	$2.64x10^{-1}$	$2.29x10^{-1}$
p-Cresol	$1.46x10^{-2}$	$2.15x10^{-2}$	$6.37x10^{-2}$	$3.50x10^{-1}$
3-Methylglutarate	$4.59x10^{-1}$	$4.66x10^{-1}$	$4.93x10^{-1}$	$4.12x10^{-1}$
N6-Acetyllysine	$5.71x10^{-1}$	$5.95x10^{-1}$	$5.46x10^{-1}$	$4.70x10^{-1}$
Acetate	1.94	1.47	1.57	3.97
Thymine	$1.73x10^{-1}$	$1.36x10^{-1}$	$1.58x10^{-1}$	$1.40x10^{-1}$
Alanine	$6.47x10^{-2}$	$6.65x10^{-2}$	$1.86x10^{-1}$	$1.85x10^{-1}$
2-Hydroxyisobutyrate	$1.04x10^{-1}$	$4.72x10^{-2}$	$3.23x10^{-2}$	$3.25x10^{-2}$
Lactate	$6.83x10^{-2}$	$1.52x10^{-1}$	$2.12x10^{-1}$	$1.46x10^{-1}$
Ethanol	$1.17x10^{-1}$	$1.09x10^{-1}$	$1.15x10^{-1}$	$1.41x10^{-1}$
Methylsuccinate	$1.34x10^{-2}$	$1.62x10^{-2}$	$1.58x10^{-2}$	$2.24x10^{-2}$
3-Hydroxyisobutyrate	$1.57x10^{-1}$	$1.52x10^{-1}$	$1.64x10^{-1}$	$1.42x10^{-1}$
Propionate	$3.04x10^{-1}$	$1.71x10^{-1}$	$1.48x10^{-1}$	$6.24x10^{-1}$
N-Isovaleroylglycine	$2.92x10^{-1}$	$2.68x10^{-1}$	$3.12x10^{-1}$	$2.77x10^{-1}$
2-Oxovalerate	$9.38x10^{-2}$	$1.35x10^{-1}$	$9.90x10^{-2}$	$1.25x10^{-1}$
Valerate	$1.68x10^{-1}$	$1.63x10^{-1}$	$2.45x10^{-1}$	$1.98x10^{-1}$