

## Supplementary Materials

# Metabolic Effect of Dietary Taurine Supplementation on Grouper (*Epinephelus coioides*): a <sup>1</sup>H NMR-based Metabolomics Study

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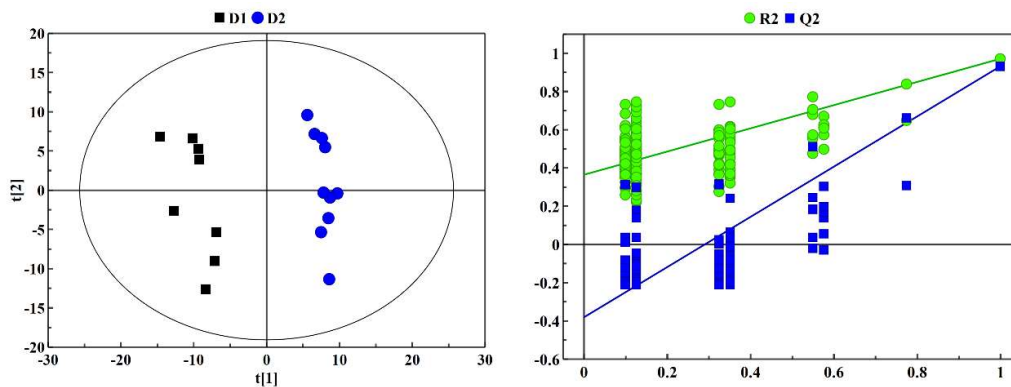
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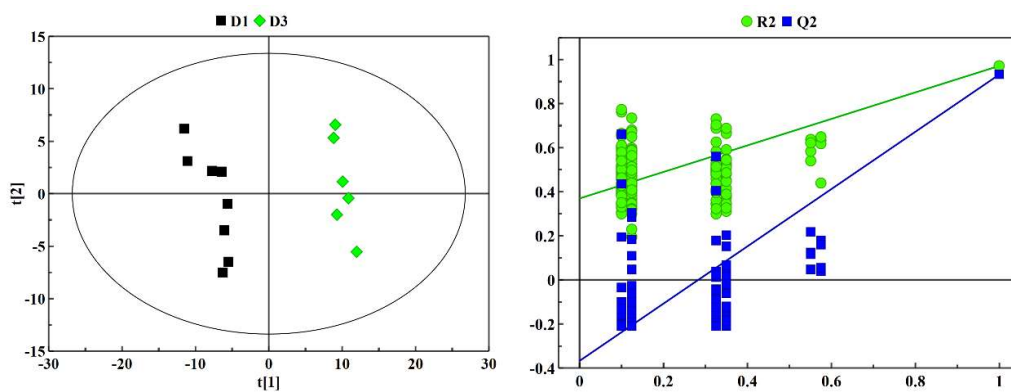
Tel./fax: +86 592 6181054.

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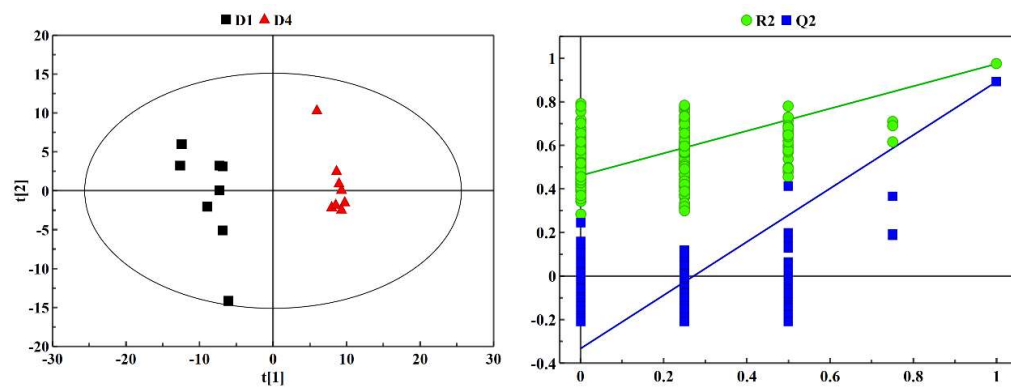
1

2 (A) D1-D2,  $R^2X=0.591$ ,  $R^2Y=0.972$ ,  $Q^2=0.932$



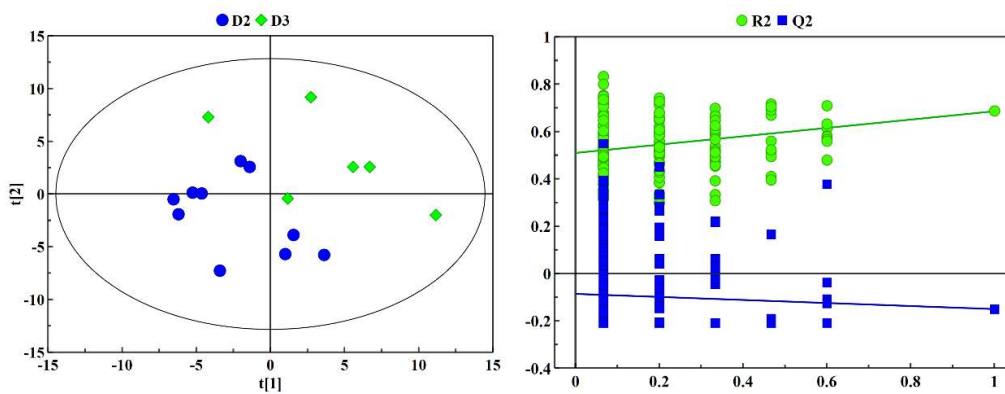
3

4 (B) D1-D3,  $R^2X=0.447$ ,  $R^2Y=0.981$ ,  $Q^2=0.875$

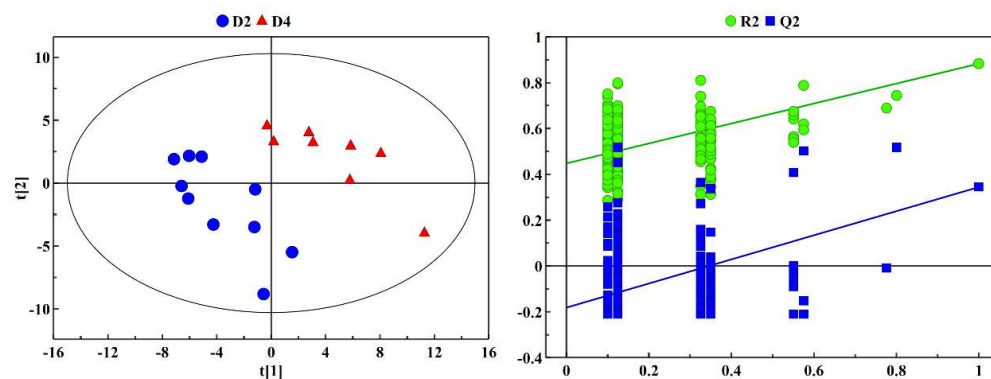


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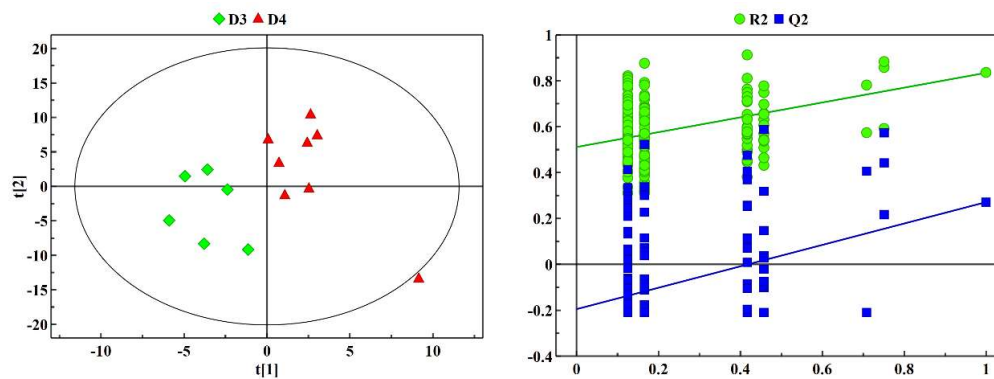
6 (C) D1-D4,  $R^2X=0.525$ ,  $R^2Y=0.974$ ,  $Q^2=0.892$



(D) D2-D3,  $R^2X=0.430$ ,  $R^2Y=0.685$ ,  $Q^2=-0.150$



(E) D2-D4,  $R^2X=0.294$ ,  $R^2Y=0.883$ ,  $Q^2=0.344$



(F) D3-D4,  $R^2X=0.467$ ,  $R^2Y=0.834$ ,  $Q^2=0.271$

**Figure S1.** PLS-DA scores plots (left panel) and validate model plots (right panel) by permutation tests ( $n=200$ ) for  $^1\text{H}$  NMR spectra of grouper intestine between different taurine-supplemented groups at FD84. (A) D1-D2; (B) D1-D3; (C) D1-D4; (D) D2-D3; (E) D2-D4; (F) D3-D4.

**Table S1** Ingredients and composition of experimental diets (on an as fed basis)

Ingredients (%)	Diets at different taurine inclusion contents			
	D1 (0.0%)	D2 (0.5%)	D3 (1.0%)	D4 (1.5%)
Casein	47	47	47	47
Gelatin	8	8	8	8
Wheat flour	24	24	24	24
Fish oil	3	3	3	3
Soybean oil	3	3	3	3
Soybean lecithin	3	4	4	4
Vitamin mix <sup>1</sup>	0.2	0.2	0.2	0.2
Mineral mix <sup>2</sup>	0.3	0.3	0.3	0.3
Vitamin C	0.02	0.02	0.02	0.02
Monocalcium phosphate	2	2	2	2
Choline chloride	0.3	0.3	0.3	0.3
Shrimp meal	3	3	3	3
Microcrystalline cellulose	3.18	2.68	2.18	1.68
Taurine	0	0.5	1.0	1.5
<b>Nutrient level (%)</b>				
Dry matter	90.81	90.76	90.24	90.21
Crude protein	49.55	49.21	49.13	49.56
Crude lipid	8.78	8.61	8.54	8.71
Ash	2.21	2.54	2.35	2.42
Taurine	0.10	0.49	0.96	1.47

<sup>1</sup> Vitamin premix consisted of (mg /kg diet) the following: vitamin A 10; vitamin D 10; vitamin K 40; vitamin E 100; vitamin B1 60; vitamin B2 70; vitamin B6 80; vitamin B12 0.4; nicotinic acid 200; calcium pantothenate 200; biotin 2; inositol 500; folic acid 8.

<sup>2</sup> Mineral premix consisted of (mg /kg diet) the following: FeSO<sub>4</sub>·7H<sub>2</sub>O 497.84, CuSO<sub>4</sub>·5H<sub>2</sub>O 11.8, ZnSO<sub>4</sub>·7H<sub>2</sub>O 175.84, MnSO<sub>4</sub>·4H<sub>2</sub>O 121.8, CoCl<sub>2</sub>·6H<sub>2</sub>O 0.18, KIO<sub>3</sub> 0.51, Na<sub>2</sub>SeO<sub>3</sub> 0.33.

24 **Table S2** Metabolites identified from NMR spectra of grouper intestine and the  
 25 corresponding assignments

Number	Metabolites	Abbreviation	HMDB ID	<sup>1</sup> H NMR chemical shift (ppm) (multiplicity) <sup>a</sup>	Assignment <sup>b</sup>
1	1-Methylhistidine	1-MH	0000001	7.06(s), 7.78(s)	CH(2), CH(4)
2	2-oxoisocaproate	2-Ox	0000695	2.61 (d)	CH <sub>2</sub>
3	3-Hydroxybutyrate	3-HB	0041603	1.20(d), 2.31(dd), 2.40(m), 4.16(m)	CH <sub>3</sub>
4	3-Methylhistidine	3-MH	0000479	7.03(s)	CH(4)
5	Acetate	Ace	0029699	1.92(s)	CH <sub>3</sub> ,
6	Adenosine	Ade	0000050	4.29(dd),4.44(dd),6.11(d), 8.37(s)	CH(2), N-CH=N
7	Adenosine monophosphate	AMP	0000045	4.52(d),6.15(d),8.27(s), 8.61(s)	CH-N, N-CH=N, N-CH'=N
8	Alanine	Ala	0028878	1.48(d)	CH <sub>3</sub>
9	Anserine	Ans	0000194	7.78 (s)	CH(4)
10	Asparagine	Asn	0029012	2.88(dd),2.95(dd),3.99(dd)	β-CH, β'-CH, α-CH
11	Aspartate	Asp	0028749	2.70(dd),2.81(dd),3.94(dd)	β-CH, β-CH', α-CH
12	Choline	Ch	0000097	3.20(s)	CH <sub>3</sub>
13	Creatine	Cr	0000064	3.04(s), 3.93(s)	CH <sub>3</sub> , CH <sub>2</sub>
14	Cytidine	Cyd	0000089	5.87(d),7.81(d)	CH(5),CH(6)
15	Dimethylamine	DMA	0000087	2.72(s)	CH <sub>3</sub>
16	Ethanolamine	EA	0000149	3.11(t),3.86(t)	CH <sub>2</sub> NH <sub>2</sub> , CH <sub>2</sub> OH
17	Formate	For	0031351	8.46(s)	CH
18	Fumarate	Fum	0031257	6.52(s)	CH
19	Glutamate	Glu	0028994	2.08(m), 2.11(m), 2.35(m), 3.75(t)	α-CH, β-CH <sub>2</sub> , γ-CH <sub>2</sub>
20	Glutamine	Gln	0028861	2.14(m), 2.45(m), 3.75(t)	γ-CH <sub>2</sub> , α-CH
21	Glycerol	G	0000131	3.55(m), 3.66(dd), 3.78(m)	CH <sub>2</sub> , CH <sub>2</sub> '
22	Glycine	Gly	0000123	3.56(s)	CH
23	Hypoxanthine	HX	0000157	8.20(s)	CH(7)
24	Inosine	Ino	0000195	4.26(dd),6.08(d),8.25(s), 8.34(s)	CH(5), CH(2), N-CH'=N
25	Isobutyrate	IB	0037189	1.07(d)	β-CH <sub>3</sub>
26	Isoleucine	Ile	0028844	0.94(t), 1.01(d),1.26(m)	δ-CH <sub>3</sub> , β-CH <sub>3</sub>
27	Lactate	Lac	0037212	1.33(d), 4.11(q)	CH <sub>3</sub> , CH
28	Leucine	Leu	0028735	0.96(t)	CH <sub>3</sub>
29	Lysine	Lys	0003405	1.46(m), 1.73(m), 1.91(m), 3.03(m), 3.76(t)	δ-CH <sub>3</sub> , β-CH <sub>3</sub> , ε-CH <sub>3</sub> , α-CH <sub>3</sub>
30	Malonate	M	0029537	3.11(s)	CH <sub>2</sub>
31	Methanol	Mol	0001875	3.36(s)	CH <sub>3</sub>
32	Methionine	Met	0002005	2.14(s), 2.63(t)	S-CH <sub>3</sub> , β-CH <sub>3</sub> , S-CH <sub>2</sub>

33	myo-Inositol	m-I	0000213	3.52(dd), 3.61(dd), 4.07(m)	CH(1), CH(2), CH(3), CH(4), CH(6)
34	Nicotinamide adenine dinucleotide	NAD	0000902	4.37(m), 4.42(m), 4.49(m), 4.51(m), 6.04(d), 6.12(d), 8.42(d), 8.83(d), 9.14(d), 9.34(s)	CH(2), CH(3), CH-OH, O-CH-N, CH(7), CH <sub>2</sub> (39)
35	Phenylalanine	Phe	0028892	4.00(m), 7.32(d), 7.37(t), 7.42(s)	o-CH, p-CH, m-CH
36	Phosphocholine	PC	0001565	3.21(s), 4.18(m)	CH <sub>3</sub>
37	Proline	Pro	0029113	3.33(m)	$\gamma$ -CH <sub>2</sub> , half $\beta$ -CH <sub>2</sub> , half $\beta$ -CH <sub>2</sub> $\delta$ -CH <sub>2</sub> , CH
38	Pyruvate	Py	0031643	2.37(s)	CH <sub>3</sub>
39	Succinate	Suc	0033837	2.40(s)	CH
40	Taurine	Tau	0000251	3.27(t), 3.42(t),	CH <sub>2</sub> SO <sub>3</sub> , NCH <sub>2</sub>
41	Trimethylamine	TMA	0000906	2.89(s)	CH <sub>3</sub>
42	Tyrosine	Tyr	0028765	6.90(d), 7.19(d)	m-CH, o-CH
43	Uracil	Uc	0000300	5.80(d), 7.55(d)	CH(5), CH(6)
44	Uridine	Ud	0000296	4.24(t), 4.36(t), 5.91(d), 5.93(d), 7.89(d)	CH(a), CH(b), CH(c), CH(5), CH(6)
45	Uridine diphosphate glucose	UDG	0000286	5.61(dd), 5.97(m), 7.96(d)	CH(2), CH(21), CH(31), N-CH=C
46	Urocanate	Urc	0000301	6.39(d), 7.38(s), 7.81(s)	CHCOOH, CH=C, CH=N
47	Valine	Val	0000883	0.99(d), 1.04(d), 2.28(m)	$\gamma$ -CH <sub>3</sub> , $\gamma$ -CH <sub>3</sub> '
48	$\alpha$ -Glucose	$\alpha$ -Glc	0062621	3.42(t), 3.54, 3.71(t), 3.73(m), 3.84(m), 5.24(d)	CH(2), CH(3), CH(5&6'), CH(1)
49	$\alpha$ -Ketoglutarate	Kg	0061388	2.45(t), 3.01(t)	$\gamma$ -CH <sub>2</sub>
50	$\beta$ -Glucose	$\beta$ -Glc	0062476	3.24(dd), 3.41(t), 3.46(m), 3.49(t), 3.90(dd)	CH(5), CH(3), CH(6), CH(1)

26 <sup>a</sup> Multiplicity: s, singlet; d, doublet; t, triplet; q, quartet; dd, doublet of doublets; m, multiplet.

27 <sup>b</sup> Assignment: according to the HMDB database ([www.hmdb.ca](http://www.hmdb.ca)).

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**Table S3** Relative concentration value (Mean  $\pm$  SD) of different metabolites by the calculation of characteristic peaks during the 84 days feeding trail

Metabolites	characteristic peaks (ppm)	FD28				FD56				FD84			
		D1	D2	D3	D4	D1	D2	D3	D4	D1	D2	D3	D4
1-Methylhistidine	7.06(s)	0.85 $\pm$ 0.20	0.76 $\pm$ 0.24	1.20 $\pm$ 0.41	1.06 $\pm$ 0.22	0.82 $\pm$ 0.13	1.05 $\pm$ 0.25	1.03 $\pm$ 0.22	1.24 $\pm$ 0.27	0.46 $\pm$ 0.21	0.60 $\pm$ 0.09	0.63 $\pm$ 0.16	0.96 $\pm$ 0.21
2-oxoisocaproate	2.61(d)	0.03 $\pm$ 0.03	0.06 $\pm$ 0.09	0.16 $\pm$ 0.18	0.10 $\pm$ 0.10	0.02 $\pm$ 0.03	0.03 $\pm$ 0.05	0.01 $\pm$ 0.03	0.03 $\pm$ 0.04	0.04 $\pm$ 0.06	0.08 $\pm$ 0.06	0.11 $\pm$ 0.11	0.04 $\pm$ 0.02
3-Hydroxybutyrate	1.20(d)	0.24 $\pm$ 0.08	0.13 $\pm$ 0.04	0.23 $\pm$ 0.13	0.95 $\pm$ 0.54	0.25 $\pm$ 0.15	0.16 $\pm$ 0.05	0.24 $\pm$ 0.07	0.15 $\pm$ 0.03	0.39 $\pm$ 0.43	0.23 $\pm$ 0.04	0.23 $\pm$ 0.09	0.27 $\pm$ 0.09
3-Methylhistidine	7.03(s)	0.85 $\pm$ 0.20	0.76 $\pm$ 0.24	1.20 $\pm$ 0.41	1.06 $\pm$ 0.22	0.82 $\pm$ 0.13	1.05 $\pm$ 0.25	1.03 $\pm$ 0.22	1.24 $\pm$ 0.27	0.46 $\pm$ 0.21	0.60 $\pm$ 0.09	0.63 $\pm$ 0.16	0.75 $\pm$ 0.21
Acetate	1.92(s)	1.55 $\pm$ 0.64	1.51 $\pm$ 0.68	1.05 $\pm$ 0.26	1.59 $\pm$ 0.54	0.71 $\pm$ 0.24	0.97 $\pm$ 0.32	0.86 $\pm$ 0.27	0.96 $\pm$ 0.22	0.90 $\pm$ 0.33	1.14 $\pm$ 0.24	0.98 $\pm$ 0.15	0.96 $\pm$ 0.18
Adenosine	8.37(s)	0.56 $\pm$ 0.74	0.54 $\pm$ 0.66	0.88 $\pm$ 0.93	0.68 $\pm$ 0.92	1.58 $\pm$ 0.73	1.83 $\pm$ 0.64	1.75 $\pm$ 1.02	1.81 $\pm$ 0.91	2.55 $\pm$ 0.41	2.79 $\pm$ 0.38	2.35 $\pm$ 1.28	2.40 $\pm$ 0.59
Adenosine monophosphate	8.61(s)	0.06 $\pm$ 0.05	0.10 $\pm$ 0.06	0.06 $\pm$ 0.04	0.09 $\pm$ 0.04	0.05 $\pm$ 0.04	0.04 $\pm$ 0.03	0.06 $\pm$ 0.06	0.05 $\pm$ 0.04	0.01 $\pm$ 0.02	0.01 $\pm$ 0.02	0.01 $\pm$ 0.01	0.01 $\pm$ 0.01
Alanine	1.48(d)	3.21 $\pm$ 0.33	2.71 $\pm$ 0.44	2.95 $\pm$ 0.62	3.59 $\pm$ 0.43	2.84 $\pm$ 0.55	3.11 $\pm$ 0.76	3.19 $\pm$ 0.64	3.45 $\pm$ 0.67	1.70 $\pm$ 0.41	2.07 $\pm$ 0.27	2.13 $\pm$ 0.28	2.19 $\pm$ 0.47
Anserine	7.78(s)	0.59 $\pm$ 0.16	0.41 $\pm$ 0.22	0.52 $\pm$ 0.43	0.64 $\pm$ 0.42	0.56 $\pm$ 0.22	0.66 $\pm$ 0.27	0.67 $\pm$ 0.30	0.78 $\pm$ 0.33	0.33 $\pm$ 0.15	0.33 $\pm$ 0.13	0.44 $\pm$ 0.22	0.48 $\pm$ 0.19
Asparagine	2.95(dd)	0.45 $\pm$ 0.33	0.66 $\pm$ 0.19	1.08 $\pm$ 0.45	0.64 $\pm$ 0.35	0.64 $\pm$ 0.13	0.76 $\pm$ 0.22	0.70 $\pm$ 0.24	0.89 $\pm$ 0.26	0.39 $\pm$ 0.10	0.41 $\pm$ 0.16	0.55 $\pm$ 0.07	0.49 $\pm$ 0.17
Aspartate	2.81(dd)	0.56 $\pm$ 0.60	0.23 $\pm$ 0.31	0.32 $\pm$ 0.46	0.58 $\pm$ 0.51	0.22 $\pm$ 0.27	0.11 $\pm$ 0.21	0.11 $\pm$ 0.14	0.10 $\pm$ 0.11	1.16 $\pm$ 0.39	0.83 $\pm$ 0.61	0.69 $\pm$ 0.48	0.31 $\pm$ 0.53
Choline	3.20(s)	1.04 $\pm$ 0.53	1.24 $\pm$ 0.70	0.92 $\pm$ 0.41	1.13 $\pm$ 0.51	1.36 $\pm$ 0.63	1.38 $\pm$ 0.67	1.34 $\pm$ 0.61	1.21 $\pm$ 0.49	1.39 $\pm$ 0.61	0.90 $\pm$ 0.57	0.68 $\pm$ 0.48	0.82 $\pm$ 0.47
Creatine	3.04(s)	5.03 $\pm$ 0.67	6.36 $\pm$ 1.74	5.40 $\pm$ 1.08	5.18 $\pm$ 0.64	6.19 $\pm$ 0.74	6.62 $\pm$ 0.63	6.67 $\pm$ 1.36	5.84 $\pm$ 1.20	5.63 $\pm$ 0.56	4.59 $\pm$ 0.68	4.53 $\pm$ 0.47	4.29 $\pm$ 0.70
Cytidine	7.81(d)	0.65 $\pm$ 0.18	0.47 $\pm$ 0.23	0.61 $\pm$ 0.45	0.71 $\pm$ 0.43	0.67 $\pm$ 0.26	0.79 $\pm$ 0.34	0.80 $\pm$ 0.34	0.93 $\pm$ 0.34	0.53 $\pm$ 0.08	0.56 $\pm$ 0.13	0.60 $\pm$ 0.24	0.67 $\pm$ 0.18
Dimethylamine	2.72(s)	0.05 $\pm$ 0.02	0.05 $\pm$ 0.01	0.05 $\pm$ 0.02	0.06 $\pm$ 0.01	0.02 $\pm$ 0.01	0.03 $\pm$ 0.01	0.02 $\pm$ 0.01	0.02 $\pm$ 0.01	0.03 $\pm$ 0.02	0.06 $\pm$ 0.03	0.05 $\pm$ 0.03	0.04 $\pm$ 0.02
Ethanolamine	3.86(t)	0.59 $\pm$ 0.19	0.73 $\pm$ 0.19	0.94 $\pm$ 0.25	0.65 $\pm$ 0.10	0.58 $\pm$ 0.21	0.51 $\pm$ 0.14	0.50 $\pm$ 0.16	0.53 $\pm$ 0.14	0.77 $\pm$ 0.20	0.66 $\pm$ 0.17	0.52 $\pm$ 0.22	0.49 $\pm$ 0.16
Formate	8.46(s)	0.53 $\pm$ 0.23	0.38 $\pm$ 0.15	0.67 $\pm$ 0.40	0.26 $\pm$ 0.12	0.08 $\pm$ 0.05	0.08 $\pm$ 0.03	0.11 $\pm$ 0.04	0.08 $\pm$ 0.02	0.08 $\pm$ 0.04	0.06 $\pm$ 0.02	0.05 $\pm$ 0.10	0.05 $\pm$ 0.04
Fumarate	6.52(s)	0.10 $\pm$ 0.04	0.10 $\pm$ 0.01	0.09 $\pm$ 0.04	0.08 $\pm$ 0.05	0.11 $\pm$ 0.03	0.13 $\pm$ 0.03	0.16 $\pm$ 0.05	0.12 $\pm$ 0.04	0.08 $\pm$ 0.01	0.08 $\pm$ 0.03	0.06 $\pm$ 0.02	0.06 $\pm$ 0.02
Glutamate	2.35(m)	6.41 $\pm$ 1.27	5.97 $\pm$ 1.19	6.57 $\pm$ 1.63	7.14 $\pm$ 1.01	5.95 $\pm$ 1.07	6.36 $\pm$ 0.94	5.86 $\pm$ 0.85	6.52 $\pm$ 0.77	5.13 $\pm$ 0.74	3.42 $\pm$ 0.58	3.56 $\pm$ 1.01	2.95 $\pm$ 0.70
Glutamine	2.45(m)	0.61 $\pm$ 0.24	0.73 $\pm$ 0.16	0.93 $\pm$ 0.21	0.70 $\pm$ 0.23	0.70 $\pm$ 0.07	0.77 $\pm$ 0.10	0.79 $\pm$ 0.19	0.81 $\pm$ 0.16	0.55 $\pm$ 0.08	0.43 $\pm$ 0.06	0.42 $\pm$ 0.04	0.35 $\pm$ 0.09
Glycerol	3.66(dd)	0.50 $\pm$ 0.34	0.61 $\pm$ 0.19	0.92 $\pm$ 0.67	0.84 $\pm$ 0.30	0.56 $\pm$ 0.25	0.58 $\pm$ 0.26	0.58 $\pm$ 0.20	0.52 $\pm$ 0.17	0.57 $\pm$ 0.29	0.36 $\pm$ 0.22	0.35 $\pm$ 0.15	0.33 $\pm$ 0.19

Glycine	3.56(s)	0.09±0.14	0.13±0.09	0.24±0.34	0.59±0.47	0.02±0.06	0.04±0.05	0.02±0.05	0.02±0.04	0.10±0.10	0.06±0.05	0.06±0.06	0.06±0.04
Hypoxanthine	8.20(s)	0.65±0.71	0.78±0.70	0.98±0.38	0.52±0.57	0.64±0.27	0.84±0.30	1.07±0.48	0.71±0.29	0.37±0.15	0.47±0.12	0.67±0.65	0.46±0.30
Inosine	8.34(s)	0.56±0.74	0.54±0.66	0.88±0.93	0.68±0.92	1.58±0.73	1.83±0.64	1.75±1.02	1.81±0.91	2.55±0.41	2.01±0.38	1.64±1.28	1.83±0.59
Isobutyrate	1.07(d)	0.03±0.02	0.01±0.01	0.02±0.01	0.02±0.01	0.02±0.02	0.02±0.00	0.02±0.01	0.02±0.01	0.03±0.03	0.03±0.02	0.03±0.01	0.03±0.01
Isoleucine	1.01(d)	1.99±0.56	1.49±0.63	2.48±1.25	2.31±0.56	1.63±0.62	1.87±0.89	2.01±1.01	2.54±1.33	0.94±0.42	1.28±0.44	1.23±0.42	1.35±0.74
Lactate	1.33(d)	13.34±1.23	14.51±2.28	14.52±1.56	12.90±0.63	12.89±2.00	14.37±1.70	14.47±0.93	14.24±1.07	12.46±0.71	15.78±0.86	19.02±1.27	15.14±1.01
Leucine	0.96(t)	3.19±0.92	2.47±1.15	2.76±0.97	3.71±0.94	2.15±0.86	2.58±1.17	2.66±1.41	3.40±1.59	1.36±0.80	1.40±0.62	1.41±0.67	1.71±1.06
Lysine	1.73(m)	1.67±0.97	1.47±0.80	2.34±1.74	2.52±1.41	1.40±0.88	1.89±1.14	1.73±1.23	2.17±1.28	0.82±0.54	0.53±0.47	0.52±0.58	0.53±0.69
Malonate	3.11(s)	0.47±0.14	0.86±0.13	0.66±0.09	0.83±0.24	0.45±0.12	0.67±0.28	0.59±0.35	0.64±0.25	0.36±0.13	0.31±0.09	0.41±0.15	0.28±0.14
Methanol	3.36(s)	0.02±0.03	0.01±0.05	0.02±0.04	0.03±0.03	0.01±0.02	0.03±0.03	0.02±0.04	0.04±0.01	0.02±0.05	0.03±0.02	0.02±0.04	0.03±0.03
Methionine	2.63(t)	0.28±0.08	0.31±0.05	0.26±0.13	0.37±0.14	0.29±0.09	0.32±0.10	0.32±0.13	0.40±0.14	0.14±0.09	0.11±0.04	0.12±0.04	0.15±0.06
myo-Inositol	4.07(m)	0.48±0.37	0.49±0.29	0.36±0.36	0.50±0.24	0.76±0.36	0.70±0.39	0.89±0.41	0.70±0.31	0.73±0.31	0.35±0.39	0.31±0.38	0.31±0.24
Nicotinamide adenine dinucleotide	6.12(d)	0.28±0.34	0.27±0.30	0.42±0.45	0.32±0.42	0.79±0.34	0.90±0.30	0.84±0.52	0.88±0.44	1.22±0.13	1.42±0.18	1.07±0.68	1.13±0.26
Phenylalanine	7.42(s)	0.48±0.11	0.38±0.19	0.48±0.17	0.59±0.12	0.38±0.12	0.45±0.19	0.46±0.23	0.60±0.29	0.20±0.09	0.28±0.09	0.28±0.07	0.31±0.18
Phosphocholine	3.21(s)	1.04±0.53	1.24±0.70	0.92±0.41	1.13±0.51	1.36±0.63	1.38±0.67	1.34±0.61	1.21±0.49	1.39±0.61	0.67±0.57	0.62±0.48	0.53±0.47
Proline	3.33(m)	1.40±0.44	1.45±0.38	1.68±0.58	1.55±0.23	1.21±0.32	1.64±0.31	1.19±0.37	1.37±0.38	0.76±0.47	0.88±0.33	0.75±0.27	0.98±0.35
Pyruvate	2.37(s)	0.89±0.21	0.89±0.18	1.03±0.33	1.03±0.12	0.87±0.21	0.93±0.15	0.81±0.14	0.95±0.13	0.69±0.11	0.85±0.12	0.75±0.18	0.74±0.13
Succinate	2.40(s)	0.04±0.04	0.03±0.03	0.01±0.02	0.04±0.02	0.03±0.03	0.02±0.01	0.01±0.01	0.02±0.01	0.01±0.01	0.02±0.01	0.02±0.01	0.01±0.01
Taurine	3.27(t)	17.80±3.22	31.52±4.51	25.69±7.32	26.27±4.21	18.27±2.64	30.26±4.17	33.94±7.62	30.00±6.88	20.42±2.26	26.87±1.95	26.51±3.51	27.75±3.75
Trimethylamine	2.89(s)	0.01±0.01	0.01±0.01	0.00±0.01	0.01±0.01	0.01±0.00	0.02±0.01	0.02±0.01	0.01±0.01	0.01±0.01	0.01±0.00	0.01±0.01	0.01±0.01
Tyrosine	6.90(d)	1.32±0.30	1.15±0.48	1.68±0.43	1.59±0.32	1.14±0.26	1.28±0.43	1.32±0.51	1.65±0.62	0.71±0.19	0.88±0.22	0.89±0.10	0.93±0.37
Uracil	7.55(d)	0.47±0.15	0.42±0.18	0.42±0.14	0.56±0.20	0.27±0.10	0.31±0.11	0.31±0.08	0.33±0.24	0.13±0.04	0.24±0.09	0.25±0.08	0.25±0.10
Uridine	7.89(d)	0.24±0.23	0.16±0.11	0.38±0.15	0.14±0.17	0.60±0.15	0.67±0.15	0.74±0.17	0.67±0.21	0.67±0.15	0.46±0.12	0.39±0.18	0.43±0.17
Uridine diphosphate glucose	7.96(d)	0.08±0.09	0.11±0.14	0.11±0.16	0.08±0.16	0.01±0.05	0.01±0.05	0.01±0.08	0.04±0.10	0.06±0.11	0.02±0.07	0.01±0.03	0.02±0.04
Urocanate	7.38(s)	0.72±0.15	0.54±0.22	0.64±0.24	0.82±0.13	0.50±0.18	0.61±0.24	0.62±0.29	0.82±0.37	0.31±0.12	0.41±0.13	0.41±0.06	0.42±0.24



Valine	0.99(d)	3.36±0.96	2.69±1.33	4.87±2.37	3.89±0.95	2.76±1.00	3.17±1.25	3.52±1.45	3.88±1.70	1.86±0.71	2.56±0.86	2.39±0.73	2.49±1.07
α-Glucose	5.24(d)	4.04±2.12	3.87±1.49	3.36±2.45	2.90±1.25	3.06±0.97	2.73±0.27	2.53±0.64	2.45±0.58	3.96±0.49	2.49±0.87	2.39±1.38	2.27±0.81
α-Ketoglutarate	3.01(t)	0.91±0.26	0.72±0.22	0.81±0.24	1.40±0.47	0.77±0.14	1.12±0.20	0.97±0.30	1.18±0.45	0.50±0.14	0.43±0.17	0.55±0.12	0.54±0.12
β-Glucose	4.67(d)	2.87±1.54	2.81±1.12	2.61±1.97	2.07±0.79	2.32±0.76	1.96±0.22	1.87±0.46	1.80±0.45	3.08±0.50	1.82±0.73	1.70±1.04	1.75±0.63

30 SD: the standard deviation

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