LC-ESI-MS/MS methodology for determination of amino acids

The aTRAQ Kit for Amino Acid Analysis of Physiological Fluids was purchased from Sciex (Framingham, MA, USA). It consisted of amine-modifying labeling aTRAQ reagent $\Delta 8$, aTRAQ internal standard set of amino acids labeled with the aTRAQ reagent $\Delta 0$, 10 % sulfosalicylic acid, borate buffer of pH 8.5, 1.2 % hydroxylamine and mobile phase modifiers – formic acid and heptafluorobutyric acid. HPLC gradient grade methanol was purchased from J.T. Baker (Center Valley, PA, USA). Deionized water obtained from Millipore Simplicity UV water purification system (Waters Corporation, Milford, MA, USA) was used.

The following protocol was used for preparation of both serum and urine samples. An aliquot of 40 μ l of the sample was added to 10 μ l of 10% sulfosalicylic acid in order to precipitate proteins. After mixing and centrifugation (10 000 x g for 2 min) the supernatant was mixed with 40 μ l of borate buffer. Next an aliquot of 10 μ l the obtained solution was labeled with aTRAQ reagent solution (aTRAQ reagent Δ 8), mixed and centrifuged. After 30 min of incubation at room temperature the labeling reaction was stopped by addition of 5 μ l 1.2% hydroxylamine solution and the sample was incubated at room temperature for 15 min. In the next step 32 μ l of the internal standard solution was added to the sample. After mixing and centrifugation the sample was evaporated in a vacuum concentrator for 15 min in order to reduce volume to about 20 μ l. Then the residue was diluted with 20 μ l of water. Each determined amino acid had its corresponding internal standard (the same amino acid labeled with the aTRAQ reagent Δ 0). Two non-proteinogenic amino acids (norleucine and norvaline) were used to evaluate the labeling efficiency and recovery.

The determination of free amino acid levels was conducted using an HPLC instrument 1260 Infinity (Agilent Technologies, Santa Clara, CA, USA) combined with a 4000 QTRAP mass spectrometer (Sciex, Framingham, MA, USA) with an electrospray ionization source. The chromatographic separation was achieved on Sciex C18 column (5 µm, 4.6 mm x 150

mm) maintained at 50 °C with a flow rate of 800 µL/min. A mobile phase gradient of eluent A (0.1% formic acid and 0.01% heptafluorobutyric acid in water) and eluent B (0.1% formic acid and 0.01% heptafluorobutyric acid in methanol) was applied. A gradient profile was the following: from 2% to 40% of B from 0 till 6 min, maintained at 40% of B for 4 min, then increased to 90% of B till 11 min and held at 90% of B for 1 min. After 12 min the gradient decreased to 2% of B. From 13 to 18 min the mobile phase composition was unaltered. The injection volume was set at 2 μ l. The ion source settings were: curtain gas, 20 psig; ion spray voltage, 4500 V; source temperature, 600 °C; ion source gas 1, 60 psig and ion source gas 2, 50 psig. The mass spectrometer operated in positive ionization mode with the following parameters: entrance potential, 10 V; declustering potential, 30 V and collision cell exit potential, 5 V. Collision energy of 30 eV was applied with the exception of cystathionine, cysteine, homocysteine, argininosuccinic acid, hydroxylysine, lysine and ornithine (50 V). The list of measured MRM transitions was contained in Table S1. Scheduled multiple reaction monitoring mode was used with nitrogen as a collision gas. A system suitability test was conducted before each batch of the samples (analysis of a standard mixture) to warm up the LC-MS/MS system and check the inter-day performance of the system. Data acquisition and processing were performed using the Analyst 1.5 software (Sciex, Framingham, MA, USA).

Amino acid	MRM transition (Q1 > Q3)				
	Analyte		Internal standard		
	Q1	Q3	Q1	Q3	
1-methylhistidine	318.2	121.1	310.2	113.1	
3-methylhistidine	318.2	121.1	310.2	113.1	
alanine	238.2	121.1	230.2	113.1	
anserine	389.2	121.1	381.2	113.1	

Table S1. MRM transitions for each amino acid and its corresponding internal standard.

argmnc323.2121.1315.2113.1arginosuccinic acid439.2121.1431.2113.1asparagine281.2121.1273.2113.1aspartic acid282.1121.1274.1113.1carnosine375.2121.1367.2113.1citrulline324.2121.1316.2113.1cystathionine519.3121.1503.3113.1cystathionine537.2121.1202.2113.1glutamic acid296.2121.1288.2113.1glutamic acid295.2121.1287.2113.1glutamine295.2121.1296.2113.1glycine224.1121.1296.2113.1homocitrulline338.2121.1330.2113.1homocystine565.3121.1272.2113.1hydroxyproline280.1121.1272.2113.1isoleucine280.2121.1272.2113.1hydroxyproline280.2121.1272.2113.1hydroxyproline280.2121.1272.2113.1phenylalanine314.2121.1306.2113.1phosphoethanolamine290.1121.1266.1113.1phosphoserine334.1121.1306.2113.1phosphoserine234.2121.1266.1113.1phosphoserine234.2121.1266.2113.1proline264.2121.1	• •	202.0	101.1	215.2	110.1
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lysine443.3121.1427.3113.1methionine298.2121.1290.2113.1ornithine429.3121.1413.3113.1phenylalanine314.2121.1306.2113.1phosphoethanolamine290.1121.1282.1113.1phosphoserine334.1121.1326.1113.1proline264.2121.1256.2113.1sarcosine238.2121.1230.2113.1taurine274.1121.1266.1113.1threonine268.2121.1260.2113.1typophan353.2121.1345.2113.1typosine330.2121.1322.2113.1valine266.2121.1302.2113.1	isoleucine	280.2	121.1	272.2	113.1
methionine298.2121.1290.2113.1ornithine429.3121.1413.3113.1phenylalanine314.2121.1306.2113.1phosphoethanolamine290.1121.1282.1113.1phosphoserine334.1121.1326.1113.1proline264.2121.1256.2113.1sarcosine238.2121.1230.2113.1serine254.2121.1246.2113.1taurine274.1121.1260.1113.1threonine268.2121.1260.2113.1typtophan353.2121.1345.2113.1typosine330.2121.1322.2113.1valine266.2121.1302.2113.1	leucine	280.2	121.1	272.2	113.1
ornithine429.3121.1413.3113.1phenylalanine 314.2 121.1 306.2 113.1 phosphoethanolamine 290.1 121.1 282.1 113.1 phosphoserine 334.1 121.1 326.1 113.1 proline 264.2 121.1 256.2 113.1 sarcosine 238.2 121.1 230.2 113.1 serine 254.2 121.1 246.2 113.1 taurine 274.1 121.1 260.1 113.1 threonine 268.2 121.1 260.2 113.1 typophan 353.2 121.1 345.2 113.1 tyrosine 330.2 121.1 322.2 113.1 valine 266.2 121.1 302.2 113.1	lysine	443.3	121.1	427.3	113.1
phenylalanine314.2121.1306.2113.1phosphoethanolamine290.1121.1282.1113.1phosphoserine334.1121.1326.1113.1proline264.2121.1256.2113.1sarcosine238.2121.1230.2113.1serine254.2121.1246.2113.1taurine274.1121.1266.1113.1threonine268.2121.1260.2113.1tryptophan353.2121.1345.2113.1tyrosine330.2121.1322.2113.1valine266.2121.1302.2113.1	methionine	298.2	121.1	290.2	113.1
phosphoethanolamine290.1121.1282.1113.1phosphoserine 334.1 121.1 326.1 113.1 proline 264.2 121.1 256.2 113.1 sarcosine 238.2 121.1 230.2 113.1 serine 254.2 121.1 246.2 113.1 taurine 274.1 121.1 266.1 113.1 threonine 268.2 121.1 260.2 113.1 tryptophan 353.2 121.1 345.2 113.1 tyrosine 330.2 121.1 322.2 113.1 valine 266.2 121.1 258.2 113.1 α -aminoadipic acid 310.2 121.1 302.2 113.1	ornithine	429.3	121.1	413.3	113.1
I > 1I > 1I > 1I > 1phosphoserine 334.1 121.1 326.1 113.1 proline 264.2 121.1 256.2 113.1 sarcosine 238.2 121.1 230.2 113.1 serine 254.2 121.1 246.2 113.1 taurine 274.1 121.1 266.1 113.1 threonine 268.2 121.1 260.2 113.1 tryptophan 353.2 121.1 345.2 113.1 tyrosine 330.2 121.1 322.2 113.1 valine 266.2 121.1 258.2 113.1 α -aminoadipic acid 310.2 121.1 302.2 113.1	phenylalanine	314.2	121.1	306.2	113.1
proline 264.2 121.1 256.2 113.1 sarcosine 238.2 121.1 230.2 113.1 serine 254.2 121.1 246.2 113.1 taurine 274.1 121.1 266.1 113.1 threonine 268.2 121.1 260.2 113.1 tryptophan 353.2 121.1 345.2 113.1 tyrosine 330.2 121.1 322.2 113.1 valine 266.2 121.1 302.2 113.1	phosphoethanolamine	290.1	121.1	282.1	113.1
sarcosine238.2121.1230.2113.1serine254.2121.1246.2113.1taurine274.1121.1266.1113.1threonine268.2121.1260.2113.1tryptophan353.2121.1345.2113.1tyrosine330.2121.1322.2113.1valine266.2121.1258.2113.1α-aminoadipic acid310.2121.1302.2113.1	phosphoserine	334.1	121.1	326.1	113.1
serine 254.2 121.1 246.2 113.1 taurine 274.1 121.1 266.1 113.1 threonine 268.2 121.1 260.2 113.1 tryptophan 353.2 121.1 345.2 113.1 tyrosine 330.2 121.1 322.2 113.1 valine 266.2 121.1 258.2 113.1 α -aminoadipic acid 310.2 121.1 302.2 113.1	proline	264.2	121.1	256.2	113.1
taurine274.1121.1266.1113.1threonine268.2121.1260.2113.1tryptophan353.2121.1345.2113.1tyrosine330.2121.1322.2113.1valine266.2121.1258.2113.1α-aminoadipic acid310.2121.1302.2113.1	sarcosine	238.2	121.1	230.2	113.1
threonine268.2121.1260.2113.1tryptophan353.2121.1345.2113.1tyrosine330.2121.1322.2113.1valine266.2121.1258.2113.1α-aminoadipic acid310.2121.1302.2113.1	serine	254.2	121.1	246.2	113.1
tryptophan353.2121.1345.2113.1tyrosine330.2121.1322.2113.1valine266.2121.1258.2113.1α-aminoadipic acid310.2121.1302.2113.1	taurine	274.1	121.1	266.1	113.1
tyrosine330.2121.1322.2113.1valine266.2121.1258.2113.1α-aminoadipic acid310.2121.1302.2113.1	threonine	268.2	121.1	260.2	113.1
valine 266.2 121.1 258.2 113.1 α-aminoadipic acid 310.2 121.1 302.2 113.1	tryptophan	353.2	121.1	345.2	113.1
α-aminoadipic acid 310.2 121.1 302.2 113.1	tyrosine	330.2	121.1	322.2	113.1
	valine	266.2	121.1	258.2	113.1
α-amino-n-butyric 252.2 121.1 244.2 113.1	α-aminoadipic acid	310.2	121.1	302.2	113.1
	α-amino-n-butyric	252.2	121.1	244.2	113.1
β-alanine 238.2 121.1 230.2 113.1	β-alanine	238.2	121.1	230.2	113.1

β-aminoisobutyric	252.2	121.1	244.2	113.1
γ-amino-n-butyric	252.2	121.1	244.2	113.1
δ-hydroxylysine	459.3	121.1	443.3	113.1