

Supporting information

A sample preparation method for simultaneous profiling signalling lipids and polar metabolites in small quantities of muscle tissues from a mouse model for sarcopenia

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Table S1. The information of lipid ISTDs.

Name	Concentration (mM)	Precursor Mass (M/Z)	Fragment Mass (M/Z)	Retention Time (min)	Class
<i>Analysed by low pH LC-MS/MS method</i>					
DCA-d4	1.00	395.3	349.1	10.2	Bile Acids & Steroid
GCA-d4	1.00	468.3	74.05	5.5	Bile Acids & Steroid
UDCA-d4	1.00	395.3	395.3	8.1	Bile Acids & Steroid
GUDCA-d5	1.00	453.3	74.1	5	Bile Acids & Steroid
SEA-d3	0.10	331.3	62.2	13.72	Endocannabinoids
OEA-d4	0.10	330.3	66.2	13.35	Endocannabinoids
PEA-d4	0.10	304.3	62.2	13.23	Endocannabinoids
2-AG-d8	0.26	387.3	294.2	13.21	Endocannabinoids
10-NO ₂ -OA-d17	2.90	343.2	183.2	13.2	Fatty acids
FA 18:1- ω 9-d17	3.34	298.1	298.1	13.8	Fatty acids
FA 22:6- ω 3-d5	1.50	332.1	288.4	13.4	Fatty acids
FA 20:4- ω 6-d8	32.00	311.1	267.2	13.47	Fatty acids
14,15-DiHETrE-d11	0.29	348.2	207.1	9.8	Oxylipins
5-iPF _{2α} -VI-d11	0.27	364.2	115.05	3.9	Oxylipins
8,12-iPF _{2α} -IV-d11	0.27	364.21	115.05	5.9	Oxylipins
12,13-DiHOME-d4	0.31	317.2	185.1	9.3	Oxylipins
8iso-PGE ₂ -d4	0.28	355.3	275.25	5.42	Oxylipins
8iso-PGF _{2α} -d4	0.28	357.3	197.15	4.75	Oxylipins
9,10-DiHOME-d4	0.31	317.2	203.1	9.5	Oxylipins
9-HODE-d4	0.33	299.2	172.1	11.1	Oxylipins
LTB ₄ -d4	0.29	339.5	197.1	9.2	Oxylipins
PGE ₂ -d4	0.28	355.3	275.25	5.42	Oxylipins
PGF _{2α} -d4	0.28	357.3	197.15	4.75	Oxylipins
TXB ₂ -d4	0.27	373.5	173.3	3.7	Oxylipins
20-HETE-d6	0.31	325.2	279.2	10.6	Oxylipins
12-HETE-d8	0.30	327.2	184.1	11.7	Oxylipins
5-HETE-d8	0.30	327.1	116.15	12.1	Oxylipins
<i>Analysed by high pH LC-MS/MS method</i>					
FA 18:1- ω 9-d17	3.34	298.2	298.2	4.311	Fatty acids
FA 22:6- ω 3-d5	1.50	332.3	288.25	4.107	Fatty acids
cLPA 17:0	2.31	405.2	269.25	5.529	Lysophospholipids & Sphingolipids
PAF 16:0	9.00	572.2	59	6.681	Lysophospholipids & Sphingolipids
LPA 17:0	14.73	423.2	153.05	4.172	Lysophospholipids & Sphingolipids
LPE 17:1	10.73	464.4	267.35	5.352	Lysophospholipids & Sphingolipids
LPI 17:1	0.57	583.4	267.3	4.589	Lysophospholipids & Sphingolipids
LPS 17:1	9.82	508.4	153.2	4.099	Lysophospholipids & Sphingolipids
Sph-1-P 17:0	2.72	366	79.05	3.596	Lysophospholipids & Sphingolipids
Sph-1-P 17:1	2.74	364	79	3.306	Lysophospholipids & Sphingolipids

Table S2. The information of amino acids and amines ISTDs.

Name	Concentration (mg/mL)	Molar (M/Z)	mass	Retention Time (min)	Class
<i>Analysed by HILIC-MS method</i>					
Asparagine- ¹³ C ₄ , ¹⁵ N ₂	0.5	137.0537		12.84	Amine
Glutamate- ¹³ C ₅ , d ₅ , ¹⁵ N	0.5	157.0911		8.38	Amino acid
Isoleucine- ¹³ C, ¹⁵ N	0.5	132.0877		7.93	Amino acid
Valine- ¹³ C ₅	0.5	121.0885		6.89	Amino acid
Leucine-d ₃	0.5	133.1062		7.64	Amino acid
<i>Analysed by CE-MS method</i>					
Aspartate- ¹³ C ₄ , d ₃ , ¹⁵ N	0.5	142.0448		14.10	Amino acid
Glutamate- ¹³ C ₅ , d ₅ , ¹⁵ N	0.5	159.0604		12.80	Amino acid
Glutamine- ¹³ C ₅	0.5	152.0764		12.70	Amine
Glycine-d ₂	0.5	78.0322		9.80	Amino acid
Isoleucine- ¹³ C, ¹⁵ N	0.5	134.0877		11.02	Amino acid
Tryptophan- ¹³ C ₁₁ , ¹⁵ N ₂	0.5	218.0972		12.50	Amino acid
Valine- ¹³ C ₅	0.5	123.0863		11.40	Amino acid

Table S3. The information of energy metabolites ISTDs.

Name	Concentration	Molar (M/Z)	mass	Retention Time (min)	Class
<i>Spiking before sample extraction (for sample extraction method evaluation)</i>					
ATP- ¹³ C ₁₀ , ¹⁵ N ₅	10 mg/mL	520.9885		12.74	Energy metabolites
AMP- ¹³ C ₁₀ , ¹⁵ N ₅	10 mg/mL	361.0558		7.07	Energy metabolites
UTP- ¹³ C ₉ , ¹⁵ N ₂	10 mg/mL	493.9613		13.90	Energy metabolites
<i>Spiking before MS analysis (only for response ratio calculation)</i>					
Fumarate-d ₂	500 mM	117.0162		13.10	Energy metabolites
Pyruvate- ¹³ C ₃	500 mM	90.0188		6.45	Energy metabolites
Succinate-d ₄	500 mM	121.0444		7.95	Energy metabolites
UMP- ¹⁵ N ₂	500 mM	325.0227		7.10	Energy metabolites

Table S4. Detected lipid metabolites in mouse muscle samples.

Name	Precursor (M/Z)	Mass	Fragment Mass (M/Z)	Retention Time (min)	ChEBI ID	ISTD	Class
<i>Analysed by low pH LC-MS/MS method</i>							
CDCA	391.2		373.25	10	16755	DCA-d4	Bile Acids & Steroid
GCA	464.2		74.1	5.5	17687	GCA-d4	Bile Acids & Steroid
GCDCA	448.21		74	8.3	36274	GUDCA-d5	Bile Acids & Steroid
GDCA	448.22		74	8.7	27471	GUDCA-d5	Bile Acids & Steroid
GUDCA	448.2		74	5	89929	GUDCA-d5	Bile Acids & Steroid
1-AG and 2-AG (two peaks merged to one)	379.21		287	13.3	34071 and 52392	2-AG-d8	Endocannabinoids
AEA	348		62	13	2700	SEA-d3	Endocannabinoids
LEA	324		62	12.9	64032	SEA-d3	Endocannabinoids
OEA	326		62	13.4	71466	OEA-d4	Endocannabinoids
PEA	300		62	13.2	71464	PEA-d4	Endocannabinoids
SEA	328		62	13.7	85299	SEA-d3	Endocannabinoids
FA16.0	255.2		237.2	13.8	15756	FA 18:1- ω 9-d17	Fatty acids
FA18.0	283.2		265.2	14.1	28842	FA 18:1- ω 9-d17	Fatty acids
FA18.1- ω 9	281.1		263.2	13.8	16196	FA 18:1- ω 9-d17	Fatty acids
FA20.3- ω 6	305.1		261	13.7	NA	FA 20:4- ω 6-d8	Fatty acids
FA20.3- ω 9	305.1		261	13.8	72865	FA 20:4- ω 6-d8	Fatty acids
FA20.4- ω 6	303		259	13.5	15843	FA 20:4- ω 6-d8	Fatty acids
FA20.5- ω 3	301.1		257.2	13.3	28364	FA 20:4- ω 6-d8	Fatty acids
FA22.6- ω 3	327.1		283.1	13.4	28125	FA 22:6- ω 3-d5	Fatty acids
10-HDoHE	343.21		153.1	11.8	72640	12-HETE-d8	Oxylipins
11-HDoHE	343.2		121.1	11.9	72794	12-HETE-d8	Oxylipins
11-HETE	319.2		167.1	11.6	72606	12-HETE-d8	Oxylipins
12,13-DiHOME	313.2		183.1	9.3	72665	12,13-DiHOME-d4	Oxylipins
12-HEPE	317.2		179.1	10.8	NA	12-HETE-d8	Oxylipins
13,14dihydro-15k-PGD ₂	351.21		175.1	6.6	72603	PGE ₂ -d4	Oxylipins
13,14dihydro-15k-PGE ₂	351.2		175.1	5.7	15550	PGE ₂ -d4	Oxylipins
13,14dihydro-PGF _{2α}	355.2		311.3	5.4	63976	PGF _{2α} -d4	Oxylipins
13-HODE	295.2		195.2	11	72639	9-HODE-d4	Oxylipins
14,15-DiHETrE	337.2		207.1	9.8	63966	14,15-DiHETrE-d11	Oxylipins
14-HDoHE	343.2		205.1	11.7	72647	12-HETE-d8	Oxylipins
15S-HETrE	321.2		221.1	12	88348	5-HETE-d8	Oxylipins
17-HDoHE	343.2		281.2	11.2	72637	12-HETE-d8	Oxylipins
18-HEPE	317.2		299.2	10.4	72802	12-HETE-d8	Oxylipins
19,20-DiHDPA	361.2		273.2	9.9	72657	14,15-DiHETrE-d11	Oxylipins
1a,1b-dihomo-PGF _{2α}	381.1		337.45	7.3	NA	PGF _{2α} -d4	Oxylipins
20-HETE	319.2		289.2	10.6	34306	20-HETE-d6	Oxylipins
5-HETE	319.2		115.15	12.3	28209	5-HETE-d8	Oxylipins
5-iPF _{2α} -VI	353.2		115.05	4	140933	5-iPF _{2α} -VI-d11	Oxylipins
7-HDoHE	343.2		281.2	12.1	72623	12-HETE-d8	Oxylipins

8-12-iso-iPF _{2α} -VI	353.21	115.05	6	NA	8,12-iPF _{2α} -IV-d11	Oxylipins
8-9-DiHETrE	337.2	127.2	10.3	63970	14,15-DiHETrE-d11	Oxylipins
8-HDoHE	343.2	189.1	12.1	72610	12-HETE-d8	Oxylipins
8-HETE	319.2	155.1	11.8	34486	5-HETE-d8	Oxylipins
8iso-15R-PGF _{2α}	353.1	193.1	3.5	NA	8iso-PGF _{2α} -d4	Oxylipins
8iso-PGE ₁	353.2	317.2	4.7	NA	8iso-PGE ₂ -d4	Oxylipins
8iso-PGE ₂	351.1	271.15	4.5	131888	8iso-PGE ₂ -d4	Oxylipins
8iso-PGF _{1α}	355.2	311.1	4.5	NA	8iso-PGF _{2α} -d4	Oxylipins
8iso-PGF _{2α}	353.1	193.1	3.7	34509	8iso-PGF _{2α} -d4	Oxylipins
8(S)-HETrE	321.2	303.2	12.3	140473	12-HETE-d8	Oxylipins
9-10-13-TriHOME	329.2	171.1	4.4	NA	12-HETE-d8	Oxylipins
9-10-DiHOME	313.2	201.05	9.6	72663	9,10-DiHOME-d4	Oxylipins
9-HEPE	317.2	167.25	10.9	89570	12-HETE-d8	Oxylipins
9-HETE	319.21	167.1	12	72786	12-HETE-d8	Oxylipins
9-HODE	295.21	171.1	11.1	72651	9-HODE-d4	Oxylipins
iPF _{2α} -IV	353.3	127.1	3.2	NA	5-iPF _{2α} -VI-d11	Oxylipins
PGD ₂	351.1	271.15	5.1	15555	PGE ₂ -d4	Oxylipins
PGD ₃	349.2	269.2	3.6	34939	PGE ₂ -d4	Oxylipins
PGE ₂	351.1	271.15	4.8	15551	PGE ₂ -d4	Oxylipins
PGF _{2α}	353.1	193.1	4.6	28031	PGF _{2α} -d4	Oxylipins
TXB ₂	369.2	169.1	3.8	15553	TXB ₂ -d4	Oxylipins

Analysed by high pH LC-MS/MS method

FA18.3-ω3	277.1	233.15	3.9	27432	FA 18:1-ω9-d17_	Fatty acids
FA22.4-ω6	331.2	287.4	5.1	NA	FA 22:6-ω3-d5	Fatty acids
FA22.5-ω3	329.2	285.4	4.7	NA	FA 22:6-ω3-d5	Fatty acids
FA22.5-ω6	329.2	285.4	4.8	NA	FA 22:6-ω3-d5	Fatty acids
cLPA16.1	389.1	253	4.7	NA	cLPA 17:0	Lysophospholipids & Sphingolipids
cLPA18.0	419.1	283	5.9	NA	cLPA 17:0	Lysophospholipids & Sphingolipids
cLPA18.1	417.2	281	5.4	62838	cLPA 17:0	Lysophospholipids & Sphingolipids
cLPA18.2	415.1	279	5	NA	cLPA 17:0	Lysophospholipids & Sphingolipids
LPA14.0	381.2	153.05	3.2	62833	LPA 17:0	Lysophospholipids & Sphingolipids
LPA16.1	407.2	153.05	3.5	75070	LPA 17:0	Lysophospholipids & Sphingolipids
LPA18.0	437.3	153.05	4.5	74850	LPA 17:0	Lysophospholipids & Sphingolipids
LPA18.1	435.2	153.05	4.1	62837	LPA 17:0	Lysophospholipids & Sphingolipids
LPA18.2	433.2	153.05	3.7	62834	LPA 17:0	Lysophospholipids & Sphingolipids
LPA20.4	457	153.05	3.9	73792	LPA 17:0	Lysophospholipids & Sphingolipids
LPA22.4	485.2	153.05	4.4	NA	LPA 17:0	Lysophospholipids & Sphingolipids
LPE14.0	424.4	196.15	4.7	NA	LPE 17:1	Lysophospholipids & Sphingolipids
LPE16.0	452.4	196.15	5.5	73134	LPE 17:1	Lysophospholipids & Sphingolipids

LPE16.1	450.4	196.15	5	NA	LPE 17:1	Lysophospholipids & Sphingolipids
LPE18.0	480.4	196.25	6.3	83047	LPE 17:1	Lysophospholipids & Sphingolipids
LPE18.1	478.4	196.25	5.7	75168	LPE 17:1	Lysophospholipids & Sphingolipids
LPE18.2	476.4	196.25	5.2	83058	LPE 17:1	Lysophospholipids & Sphingolipids
LPE18.3	474.4	196.25	4.9	NA	LPE 17:1	Lysophospholipids & Sphingolipids
LPE20.3	502.4	196.15	5.6	NA	LPE 17:1	Lysophospholipids & Sphingolipids
LPE20.4	500.4	196.15	5.3	64395	LPE 17:1	Lysophospholipids & Sphingolipids
LPE20.5	498.4	196.15	4.9	NA	LPE 17:1	Lysophospholipids & Sphingolipids
LPE22.4	528.4	196.15	5.9	NA	LPE 17:1	Lysophospholipids & Sphingolipids
LPE22.5	526.4	196.15	5.5	NA	LPE 17:1	Lysophospholipids & Sphingolipids
LPE22.6	524.4	196.15	5.3	72747	LPE 17:1	Lysophospholipids & Sphingolipids
LPG14.0	455.1	227.3	4.1	73092	LPI 17:1	Lysophospholipids & Sphingolipids
LPG16.0	483.1	255.3	4.9	75376	LPI 17:1	Lysophospholipids & Sphingolipids
LPG16.1	481.1	253.3	4.3	138795	LPI 17:1	Lysophospholipids & Sphingolipids
LPG18.0	511.1	283.3	5.5	73091	LPI 17:1	Lysophospholipids & Sphingolipids
LPG18.1	509.1	281.3	5	72952	LPI 17:1	Lysophospholipids & Sphingolipids
LPG18.2	507.1	279.3	4.6	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPG20.3	533.1	305.3	5	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPG20.4	531.1	303.3	4.8	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPG22.4	559.1	331.3	5.2	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPI16.1	569.1	253.25	4.3	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPI18.0	599.1	283.25	5.4	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPI18.1	597.1	281.25	4.8	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPI18.2	595.1	153.05	4.5	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPI20.4	619.1	303.25	4.6	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPI22.4	647.2	331.2	5.1	NA	LPI 17:1	Lysophospholipids & Sphingolipids
LPI22.6	643.2	327.2	4.6	138564	LPI 17:1	Lysophospholipids & Sphingolipids
LPS18.1	522.4	153.1	4.4	52649	LPS 17:1	Lysophospholipids & Sphingolipids
LPS18.2	520.1	153.05	4.1	NA	LPS 17:1	Lysophospholipids & Sphingolipids
LPS20.4	544.1	153.05	4.1	85435	LPS 17:1	Lysophospholipids & Sphingolipids

LPS22.4	572.1	153.05	4.6	NA	LPS 17:1	Lysophospholipids & Sphingolipids
LPS22.6	568.1	153.05	4.1	NA	LPS 17:1	Lysophospholipids & Sphingolipids

(Note: NA means nothing found).

Table S5. Detected polar metabolites in mouse muscle samples.

Metabolites name	ChEBI ID	Molar mass (M/Z)	Retention time (min)	ISTD	Class
<i>Analysed by HILIC-MS method (negative ionization mode)</i>					
6-phosphogluconic acid	48928	275.0174	10.1	Fumarate-d ₂	Energy metabolites
Acetyl-CoA	15351	808.1185	7.4	Fumarate-d ₂	Energy metabolites
Adenosine	16335	266.0889	3.8	Pyruvate- ¹³ C ₃	Energy metabolites
ADP	16761	426.0221	9.4	AMP- ¹³ C ₁₀ , ¹⁵ N ₅	Energy metabolites
AMP	16027	346.0558	7.0	AMP- ¹³ C ₁₀ , ¹⁵ N ₅	Energy metabolites
Ascorbic acid	29073	175.0242	6.7	Valine- ¹³ C ₅	Energy metabolites
ATP	15422	505.9885	11.5	ATP- ¹³ C ₁₀ , ¹⁵ N ₅	Energy metabolites
cAMP	17489	328.0452	5.7	UMP- ¹⁵ N ₂	Energy metabolites
CDP	17239	402.0109	10.7	UMP- ¹⁵ N ₂	Energy metabolites
cis-Aconitate	16383	173.0085	6.7	Valine- ¹³ C ₅	Energy metabolites
CMP	17361	322.0446	8.8	UMP- ¹⁵ N ₂	Energy metabolites
CTP	17677	481.9772	13.0	UMP- ¹⁵ N ₂	Energy metabolites
Cytidine	17562	242.0776	5.7	Leucine-d ₃	Energy metabolites
Dihydroxyacetone-P	16108	168.9907	9.1	Fumarate-d ₂	Energy metabolites
Fructose-6-P	78697	259.0224	9.6	Fumarate-d ₂	Energy metabolites
GABA	16865	102.0561	10.6	Asparagine- ¹³ C ₄ , ¹⁵ N ₂	Amino acid
GDP	17552	442.0171	13.3	UMP- ¹⁵ N ₂	Energy metabolites
Glucose	17234	179.0561	7.5	Fumarate-d ₂	Energy metabolites
Glucose-1-P	58601	259.0224	9.1	Fumarate-d ₂	Energy metabolites
Glucose-6-P	14314	259.0224	10.2	Fumarate-d ₂	Energy metabolites
Glyceraldehyde-3-P	17138	168.9907	8.4	Fumarate-d ₂	Energy metabolites
Glycerate-3-P	58272	184.9857	9.2	Fumarate-d ₂	Energy metabolites
GMP	NA	362.0507	8.9	UMP- ¹⁵ N ₂	Energy metabolites
GTP	15996	521.9834	13.6	UMP- ¹⁵ N ₂	Energy metabolites
Guanosine	16750	282.0838	6.1	Isoleucine- ¹³ C, ¹⁵ N	Energy metabolites
Hypoxanthine	17368	135.0306	4.1	Pyruvate- ¹³ C ₃	Energy metabolites
IMP	17202	347.0398	7.9	UMP- ¹⁵ N ₂	Energy metabolites
Inosine	17596	267.0728	5.4	Leucine-d ₃	Energy metabolites
Malate	25115	133.0142	7.1	Fumarate-d ₂	Energy metabolites
Oxogluthathione	167606	611.1441	11.8	Asparagine- ¹³ C ₄ , ¹⁵ N ₂	Energy metabolites
Phosphoenolpyruvate	18021	166.9751	8.9	Asparagine- ¹³ C ₄ , ¹⁵ N ₂	Energy metabolites
Pyruvate	15361	87.0088	3.7	Pyruvate- ¹³ C ₃	Energy metabolites
Succinic acid	15741	117.0193	5.8	Succinate-d ₄	Energy metabolites
UDP	17659	402.9949	9.6	UMP- ¹⁵ N ₂	Energy metabolites
UMP	28895	323.0286	7.2	UMP- ¹⁵ N ₂	Energy metabolites
Uridine	16704	243.0616	4.3	Pyruvate- ¹³ C ₃	Energy metabolites

UTP	15713	482.9613	11.6	UTP- ¹³ C ₉ , ¹⁵ N ₂	Energy metabolites
Xanthine	15318	151.0255	3.9	Pyruvate- ¹³ C ₃	Energy metabolites
α-Ketoglutarate	80619	145.0142	6.7	Fumarate-d ₂	Energy metabolites
Tyrosine	18186	180.0666	7.4	Valine- ¹³ C ₅	Amino acid
Alanine	15570	90.0550	8.9	Glutamate- ¹³ C ₅ , d ₅ , ¹⁵ N	Amino acid
Phenylalanine	28044	164.0717	5.6	Leucine-d ₃	Amino acid
Asparagine	17196	131.0462	9.8	Asparagine- ¹³ C ₄ , ¹⁵ N ₂	Amine
Leucine	25017	130.0874	5.8	Leucine-d ₃	Amino acid
Ornithine	18257	131.0826	10.5	Asparagine- ¹³ C ₄ , ¹⁵ N ₂	Amino acid
<i>Analysed by CE-MS method (positive ionization mode)</i>					
Creatine	16919	132.0768	9.6	Glycine-d ₂	Energy metabolites
Arginine	29016	175.1190	7.6	Valine- ¹³ C ₅	Amino acid
Spermidine	16610	146.1652	4.5	Glutamine- ¹³ C ₅	Amine
Aspartic acid	17364	134.0448	14.1	Aspartate- ¹³ C ₄ , d ₃ , ¹⁵ N	Amino acid
Lysine	18019	147.1190	7.2	Valine- ¹³ C ₅	Amino acid
Valine	27266	118.0863	11.4	Valine- ¹³ C ₅	Amino acid
Methionine	16811	150.0583	12.8	Isoleucine- ¹³ C, ¹⁵ N	Amino acid
Glutamine	28300	147.0764	12.7	Glutamine- ¹³ C ₅	Amine
Serine	17822	106.0499	11.8	Aspartate- ¹³ C ₄ , d ₃ , ¹⁵ N	Amino acid
Threonine	16857	120.0655	12.3	Aspartate- ¹³ C ₄ , d ₃ , ¹⁵ N	Amino acid
Glutamic acid	18237	148.0604	12.8	Glutamate- ¹³ C ₅ , d ₅ , ¹⁵ N	Amino acid
Glycine	15428	76.0393	9.8	Glycine-d ₂	Amino acid
Histidine	27570	156.0768	7.7	Valine- ¹³ C ₅	Amino acid
Tryptophan	16828	205.0972	12.5	Tryptophan- ¹³ C ₁₁ , ¹⁵ N ₂	Amino acid
4-Hydroxyproline	20392	132.0655	9.3	Valine- ¹³ C ₅	Amino acid
Proline	26271	116.0706	13.3	Valine- ¹³ C ₅	Amino acid
Creatinine	16737	114.0662	6.8	Glycine-d ₂	Amine

(Note: NA means nothing found).