Reprogrammed arachidonic acid metabolism by α-terpineol to alleviate asthma: insights from metabolomics

Ying Rong¹, Fanglin Liu¹, Hui Zhou¹, Tong Yu¹, Zhaolong Qin¹,

Qianwen Cao¹, Luyao Liu¹, Xiaoge Ma¹, Lingbo Qu¹, Peirong Xu¹,

Xinglin Liao³, Qiman Jiang³, Nan Zhang^{2*}, Xia Xu^{1*}

¹ Department of Medical Analysis, School of pharmaceutical science,

Zhengzhou University, Zhengzhou, Henan, 450001

² Department of Pharmaceutics, School of pharmaceutical science,

Zhengzhou University, Zhengzhou, Henan, 450001

³ Nanyang LANHAISENYUAN Medical technology ltd.,CO. Nanyang,

Henan, 473000

*Co-corresponding Authors:

1. Xia Xu, Department of Medical Analysis, School of pharmaceutical science, Zhengzhou University, Zhengzhou, Henan, 450001, P. R. China Tel.: 86-0371-67781911; E-mail: xuxia@zzu.edu.cn

 Nan Zhang, Department of Pharmaceutics, School of pharmaceutical science, Zhengzhou University, Zhengzhou, Henan, 450001, P. R. China Tel.: 86-0371-67781911; E-mail: nanzhang@zzu.edu.cn

Supplementary material

 Table S1 Major differential compounds and change trend in mouse lung tissue samples.

Table S2 Major differential compounds and their specific information inmouse lung tissue samples.

 Table S3 Major differential compounds and change trend in mouse serum samples.

 Table S4 Major differential compounds and their specific information in mouse serum samples.

Table S5 Summary of results of pathway analysis of differentialmetabolites in lung tissue samples.

 Table S6 Results of enrichment analysis of major differential compounds

 in mouse lung tissue samples.

Table S7 Summary of results of pathway analysis of differentialmetabolites in serum samples.

Table S8 Results of enrichment analysis of major differential compounds

 in mouse serum samples.

Fig S1 The representative total ion chromatograms (TICs) of lung tissue samples in both positive (ESI⁺) and negative (ESI⁻) ion modes.

Fig S2 The representative total ion chromatograms (TICs) of serum samples in both positive (ESI⁺) and negative (ESI⁻) ion modes.

Fig S3 The PCA analysis of QCs samples of lung tissue and serum

samples in both positive (ESI⁺) and negative (ESI⁻) ion modes.

Fig S4 MS/MS spectrum of the differential metabolites in lung tissues detected by UPLC-MS/MS.

Fig S5 MS/MS spectra of different metabolites in serum detected by UPLC-MS/MS.

Differential	Rt	,	F 1		Ion	Fold	Fold change	
compound	(min)	m/z	Formula	Adducts	Mode	M vs. C	Ter vs. M	
Arachidonic acid	19.07	303.2330		[M-H]- [M-H]-	ESI-	1.63 🕇	0.50 ↓	
LTB4	16.61	335.2228		[M-H]- [M+H]+	ESI-	1.64 🕇	0.81 ↓	
LTD4	19.20	495.2534		[M+H]+ [M+H]+	ESI-	2.46 🕇	0.28 ↓	
5-HPETE	9.72	337.2373	C20H32O2 C20H32O4	[M+H]+ [M+H]+	ESI ⁺	1.64 🕇	0.57 ↓	
L-Tryptophan	3.68	205.0972	C25H40N2O6S C20H32O4	[M-H]- [M-H]-	ESI ⁺	1.38 🕇	0.87 ↓	
Hypoxanthine	1.41	137.0458	C11H12N2O2 C5H4N4O	[M+H]+ [M+H]+	ESI ⁺	1.86 🕇	0.42 ↓	
Ornithine	0.85	133.0972	C5H12N2O2 C6H9N3O2	[M-H]- [M-H]-	ESI ⁺	3.60 🕇	0.75 ↓	
Histidine	0.86	156.0768	C20H30O2 C9H12N2O6	[M-H]- [M+H]+	ESI^+	1.67 🕇	0.81 ↓	
Abietic acid	1.03	301.2173	C4H4N2O2 C20H32O5	[M+H]+ [M+H]+	ESI-	1.74 🕇	0.72 ↓	
Uridine	1.24	243.0623	C20H32O3 C18H30O2	[M+H]+ [M+H]+	ESI-	2.16 🕇	0.57 ↓	
Uracil	1.40	113.0346	C18H32O2 C10H12N2O3	[M+H]+ [M+H]+	ESI^+	1.62 🕇	0.86 🖌	
LXA4	8.55	353.2322	C5H4N4O2 C10H13N5O4	[M+H]+ [M-H]-	ESI^+	0.64 ↓	1.38 🕇	
5-HETE	17.52	319.2279	C10H12N4O5 C10H17N3O6S	[M+H]+ [M-H]-	ESI-	0.82 ↓	1.37 🕇	
α-Linolenic acid	18.66	277.2173	C5H7NO3 C5H9N3		ESI-	0.89 ↓	1.24 🕇	
Linoleic acid	19.02	279.2330	C5H5N5 C5H4N4O3		ESI-	0.79 ↓	1.32 🕇	
Kynurenine	2.15	209.0921	C20H32O5 C20H32O5		ESI ⁺	0.76 ↓	1.64 🕇	
Xanthine	1.40	153.0407			ESI ⁺	0.74 ↓	1.18 🕇	
Adenosine	1.41	268.1040			ESI ⁺	0.81 ↓	1.23	
Inosine	1.46	269.0880			ESI^+	0.78 ↓	1.23 🕇	

Table S1 Major differential compounds and change trend in mouse lungtissue samples.

Glutathione	7.76	308.0911	ESI^+	0.18 ↓	2.94 🕇
Pyroglutamic acid	1.41	130.0499	ESI^+	0.48 ↓	1.29 🕇
Histamine	0.81	112.0869	ESI^+	0.69 ↓	1.12 🕇
				0.65 ↓	1.56 🕇
Adenine	3.01	136.0618	ESI^+		1
Uric acid	0.88	167.0210	ESI ⁻	2.18 †	0.54 ↓
PGD2	8.55	353.2322	\mathbf{ESI}^+		1 45 🛦
TXA2	12.92	351.2178	ESI ⁻	0.62 ¥	1.45 f
				1.89 🕇	0.43 ↓

Rt represents the retention time of the compound.

Table S2 Major differential compounds in mouse lung tissue samples and

Differential compound	Annotation level	CV in QCs (%)	P-V M vs C	<i>P</i> -Value M vs C Ter vs M		cted <i>P</i> - lue ^{Cer vs M}	Biochemical class	
Arachidonic acid	Level 2	13.6	< 0.01	< 0.01	0.05	0.02	Fatty acids	
LTB4	Level 2	19.7	0.01	0.02	0.05	0.22	Unsaturated acid	
LTD4	Level 2	15.4	< 0.01	< 0.01	0.01	< 0.01	Unsaturated acid	
5-HPETE	Level 2	13.5	0.02	0.02	0.05	0.21	Hydroperoxyeicosatetr aenoic acids	
L-Tryptophan	Level 2	18.9	< 0.01	0.01	< 0.01	0.11	Alpha-amino acid	
Hypoxanthine	Level 2	8.9	< 0.01	< 0.01	0.38	0.38	Purines	
Ornithine	Level 2	19.9	< 0.01	0.02	< 0.01	0.02	L-alpha-amino acids	
Histidine	Level 2	6.7	< 0.01	0.02	< 0.01	0.02	Alpha-amino acid	
Abietic acid	Level 2	4.2	0.03	0.01	0.05	0.17	Diterpenoids	
Uridine	Level 2	17.0	< 0.01	0.01	< 0.01	0.59	Pyrimidine nucleosides	

their specific information.

Uracil	Level 2	18.3	0.03	0.03	0.04	0.38	Pyrimidones	
LXA4	Level 2	12.1	< 0.01	0.03	< 0.01	0.05	Eicosanoid chemical	
							mediators	
5-HETE	Level 2	19.9	0.03	0.01	0.31	0.05	Eicosanoid	
α-Linolenic acid	Level 2	13.5	0.05	< 0.01	0.59	0.03	Omega-3 fatty acid	
Linoleic acid	Level 2	17.3	0.05	0.03	0.05	0.03	Omega-6 fatty acid	
Kynurenine	Level 2	16.4	0.04	0.04	0.44	0.04	Alkyl-phenylketone	
Xanthine	Level 2	12.0	< 0.01	0.01	0.01	0.19	Xanthines	
Adenosine	Level 2	19.8	0.05	0.01	0.05	0.12	Nucleoside	
Inosine	Level 2	13.4	0.04	0.10	0.04	0.10	Purine nucleosides	
Glutathione	Level 2	18.8	< 0.01	0.03	< 0.01	0.03	Tripeptide	
Pyroglutamic acid	Level 2	18.8	< 0.01	0.19	< 0.01	0.19	Amino acid derivative	
Histamine	Level 2	19.4	< 0.01	0.28	< 0.01	0.28	Amine	
Adenine	Level 2	10.1	0.02	0.01	0.03	0.19	6-Aminopurines	
Uric acid	Level 2	19.5	< 0.01	0.01	< 0.01	0.02	Heterocyclic purine	
							derivative	
PGD2	Level 2	16.2	0.04	0.02	0.04	0.24	Prostaglandin	
TXA2	Level 2	17.7	< 0.01	0.01	0.01	0.02	Thromboxane	

Table S3 Major differential compounds and change trend in mouse serum samples.

Differential	Rt	100 /7	Formula	Adducto	Ion	Fold	change
compound	(min)	m/z,	rormuta	Auducts	Mode	M vs. C	Ter vs. M
Arginine	0.84	175 1100	C6H14N4O2	[M+H]+	ECI+	1.22	0.00
	0.84	1/3.1190		[M+H]+	ESI	1.32 Ť	0.60
Kynurenine	2 1 1	200 0021	C10H12N2O3	[M+H]+	ESI ⁺ 1.22	1.00	
	2.11	209.0921		[M+H]+	LOI	1.22 Ť	0.60
Glutamate	1.06	148 0604	C5H9NO4	[M+H]+	ESI+	1.00	0.40
	1.00	146.0004		[M+H]+	LSI	1.22 †	0.42
Uric acid	1 2 2	160 0256	C5H4N4O3	[M+H]+	ESI+	1.02	0.40
	1.55	109.0550		[M-H]-	ESI	1.83 T	0.43
LTA4	11 12	210 2267	C20H30O3	[M-H]-	ECI+	a c o k	0.45
	11.13	519.2207		[M+H]+	ESI	2.50 T	0.45
Histidine	0.92	156 0769	C6H9N3O2	[M+H]+	ECI+		
	0.82	130.0708		[M+H]+	E21,	1.30 †	0.36

Histamine	0.79	112.0869	C5H9N3	[M-H]- [M-H]-	ESI^+	1.30 🕇	0.34↓
Arachidonic acid	19.04	303.2330	C20H32O2	[M+H]+	ESI-	2.03	0.33 🖡
Uridine	1.22	243.0623	C9H12N2O6		ESI-	1.66 🕇	0.45 ↓
Xanthine	1.34	153.0407	C5H4N4O2		ESI ⁺	0.36↓	6.60 🕇
Tryptophan	3.67	205.0972	C11H12N2O2		ESI ⁺	0.71 ↓	1.38 🕇
5-HPETE	9.72	337.2373	C20H32O4		ESI ⁺	0.39 ↓	2.37 🕇
α-Linolenic acid	18.50	277.2173	C18H30O2		ESI-	0.18 ↓	3.98 🕇
linoleic acid		279.2330	C18H32O2			1	
Valine	18.97	118.0863	C5H11NO2		ESI-	0.62 ¥	1.89 †
	1.35				ESI+	0.57 ↓	2.05

Rt represents the retention time of the compound.

Table S4 Major differential compounds in mouse serum samples andtheir specific information.

Differential	Annota	CV in	P -Value		Correc	ted <i>P</i> -valu	e Biochemical
compound	tion level	QCs (%)	M vs C	M vs C Ter vs M		C Ter vs M	class
Arginine	Level 2	5.2	< 0.01	0.02	0.04	0.05	L-alpha-amino acids
Kynurenine	Level 2	19.0	0.01	0.12	0.05	0.19	Alkyl-phenylketone
Glutamate	Level 2	17.9	0.03	< 0.01	0.12	< 0.01	Alpha-amino acid
Uric acid	Level 2	9.3	< 0.01	< 0.01	0.04	0.06	Heterocyclic purine
							derivative
LTA4	Level 2	16.3	< 0.01	< 0.01	< 0.01	< 0.01	Leukotrienes
Histidine	Level 2	19.3	< 0.01	< 0.01	0.05	< 0.01	Alpha-amino acid
Histamine	Level 2	15.5	< 0.01	0.02	0.18	0.02	Amine
Arachidonic acid	Level 2	20.0	< 0.01	0.02	< 0.01	0.02	Fatty acids
Uridine	Level 2	19.5	< 0.01	0.24	0.04	0.24	Pyrimidine nucleosides
Xanthine	Level 2	19.6	< 0.01	0.01	< 0.01	0.01	Xanthines
Tryptophan	Level 2	7.3	< 0.01	0.01	0.05	0.01	Alpha-amino acid
5-HPETE	Level 2	12.8	< 0.01	0.03	< 0.01	0.03	Hydroperoxyeicosatetr
							aenoic acids
α-Linolenic acid	Level 2	13.2	< 0.01	0.01	< 0.01	0.01	Omega-3 fatty acid
linoleic acid	Level 2	19.2	< 0.01	< 0.01	0.03	0.08	Omega-6 fatty acid
Valine	Level 2	19.5	< 0.01	< 0.01	< 0.01	< 0.01	Alpha-amino acid

Table S5 Summary of results of pathway analysis of differentialmetabolites in lung tissue.

Dothway Nama	Match		FDD	Impost	
	Status	р	ГDК	impact	
Arachidonic acid	7/26	5 17((F 7	4 2 4 9 4 E 7	0 4 6 4 4	
metabolism	//30	3.1/00E-/	4.3484E-7	0.4644	
Purine metabolism	6/65	0.2004E-4	0.010454	0.00754	
Glutathione metabolism	3/28	0.0082928	0.2322	0.26305	
Biosynthesis of unsaturated	2/20	0.01((()	0.24090	0.0	
fatty acids	3/30	0.016662	0.34989	0.0	
Histidine metabolism	2/16	0.024162	0.40592	0.40983	
beta-Alanine metabolism	2/21	0.040341	0.56477	0.0	
Linoleic acid metabolism	1/5	0.075153	0.90183	1.0	

Table S6 Results of enrichment analysis of major differential compoundsin mouse lung tissue samples.

Metabolite Set	Total	Hits	Expect	P value	FDR
Arachidonic acid metabolism	69	8	1.62	8.76E-5	0.00858
Purine metabolism	74	6	1.73	0.00549	0.269
Alpha-linolenic and linoleic acid	19	3	0 445	0 00858	0.28
metabolism	19	5	0.443	0.00858	0.28
Glutathione metabolism	21	2	0.492	0.0843	1.0

Table S7 Summary of results of pathway analysis of differentialmetabolites in serum.

Dathway Nama	Match	D	FND	Impost	
Fathway Mame	Status	ſ	ГDK	Impact	
Aminoacyl-tRNA	5/40	5 4005E 5	0.004(101	0.0	
biosynthesis	5/48	3.4905E-3	0.0046121	0.0	
Histidine metabolism	3/16	3.8127E-4	0.016013	0.40983	
Biosynthesis of unsaturated	2/26	0.0042244	0.000012	0.0	
fatty acids	3/36	0.0043244	0.090813	0.0	
Arachidonic acid	2/26	0.0042244	0.000012	0.40(12	
metabolism	3/36	0.0043244	0.090813	0.49613	
Arginine biosynthesis	2/14	0.0074414	0.12502	0.19289	
Linoleic acid metabolism	1/5	0.04752	0.48448	1.0	
Arginine and proline	2/20	0.050270	0 40 4 40	0 1 4 2 9 6	
metabolism	2/38	0.050279	0.48448	0.14386	

Table S8 Results of enrichment analysis of major differential compoundsin mouse serum samples.

Metabolite Set	Totol	Hits	Expect	P value	FDR
Alpha-linolenic and linoleic	19	3	0.278	0.00214	0.21
acid metabolism					
Arachidonic acid metabolism	69	4	1.01	0.0146	0.717
Histidine metabolism	43	3	0.63	0.0221	0.721
Trytophan metabolism	60	3	0.879	0.0526	0.884
Methylhistidine Metabolism	4	1	0.0586	0.0574	0.884
Urea cycle	29	2	0.425	0.0647	0.884
Ammonia Recycling	32	2	0.469	0.0771	0.884

Fig S1 The representative total ion chromatograms (TICs) of lung tissue samples in ESI⁺ and ESI⁻ modes.



Fig S2 The representative total ion chromatograms (TICs) of serum samples in ESI⁺ and ESI⁻ modes.



Fig S3 The PCA analysis of QCs samples of lung tissue and serum samples in both positive (ESI⁺) and negative (ESI⁻) ion modes.





Fig S4 MS/MS spectra of different metabolites in lung tissues detected by UPLC-MS/MS.

1.Arachidonic Acid (AA)

[M-H] :303.2329



MS/MS spectrum of arachidonic acid detected in mouse lung tissue





351

MS/MS spectrum of arachidonic acid from MassBank

Arachidonic acid; LC-ESI-QTOF; MS2; CE:20 eV; [M-H]-



2.Thromboxane A2 (TXA2)

[M-H] :351.2176



MS/MS spectrum of TXA2 detected in mouse lung tissue

MS/MS spectrum of TXA2 from HMDB



[M-H] :335.2227





MS/MS spectrum of LTB4 from HMDB



[M-H] :495.2534



MS/MS spectrum of LTD4 detected in mouse lung tissue

MS/MS spectrum of LTD4 from HMDB



[M+H]:337.2373

MS/MS spectrum of 5-HPETE detected in mouse lung tissue



MS/MS spectrum of 5-HPETE from HMDB



[M+H]:205.0971



MS/MS spectrum of L-Tryptophan detected in mouse lung tissue

MS/MS spectrum of L-Tryptophan from mzCloud



MS/MS spectrum of L-Tryptophan from Mass Bank

L-Tryptophan; LC-ESI-QTOF; MS2; CE 20 ev; [M+H]+



7.Hypoxanthine

[M+H]:137.0457

MS/MS spectrum of Hypoxanthine detected in mouse lung tissue



MS/MS spectrum of Hypoxanthine from mzCloud



8. Ornithine

[M+H]:133.0971



MS/MS spectrum of Ornithine detected in mouse lung tissue

MS/MS spectrum of Ornithine from mzCloud



MS/MS spectrum of Ornithine from MassBank

L-Ornithine; ESI-QTOF; MS2; POSITIVE; [M+H]+; CID; 10 V

Mass S	pectrum
e	800.0
dano	600.0

133.0955

9. Histidine

[M+H]:156.0767



MS/MS spectrum of Histidine detected in mouse lung tissue

MS/MS spectrum of Histidine from mzCloud



[M-H]: 301.2173



MS/MS spectrum of Abietic acid detected in mouse lung tissue

MS/MS spectrum of Abietic acid from mzCloud



MS/MS spectrum of Abietic acid from MassBank

Abietic acid; LC-ESI-QTOF; MS2; CE 20 ev; [M-H]-



11.Uridine

[M-H] :243.0622



MS/MS spectrum of Uridine detected in mouse lung tissue

MS/MS spectrum of Uridine from mzCloud



MS/MS spectrum of Uridine from MassBank



Uridine; LC-ESI-QTOF; MS2; CE: 20; R=; [M-H]-

[M+H]:113.0345



MS/MS spectrum of Uracil detected in mouse lung tissue

MS/MS spectrum of Uracil from HMDB



MS/MS spectrum of Uridine from MassBank



Uracil; LC-ESI-QTOF; MS2; CE:Ramp 5-60 V; [M+H]+

13. Lipoxin A4 (LXA4)

[M+H]:353.2322

MS/MS spectrum of LXA4 detected in mouse lung tissue



MS/MS spectrum of LXA4 from HMDB



14.5-HETE

[M-H] :319.2278

MS/MS spectrum of 5-HETE detected in mouse lung tissue



MS/MS spectrum of 5-HETE from HMDB



15.α-Linolenic acid





MS/MS spectrum of α-Linolenic acid detected in mouse lung tissue

MS/MS spectrum of α -Linolenic acid from HMDB



16. Linoleic acid





MS/MS spectrum of Linoleic acid detected in mouse lung tissue





MS/MS spectrum of Linoleic acid from MassBank



Linoleic acid; LC-ESI-QTOF; MS2; CE: 20; R=; [M-H]-

17.Kynurenine

[M+H]: 209.0920





MS/MS spectrum of Kynurenine from HMDB



MS/MS spectrum of Kynurenine from MassBank



Kynurenine; LC-ESI-QTOF; MS2; [M+H]+; CE: 10eV

18.Xanthine

[M+H]:153.0407

MS/MS spectrum of Xanthine detected in mouse lung tissue



MS/MS spectrum of Xanthine from mzCloud



MS/MS spectrum of Xanthine from MassBank



Xanthine; LC-ESI-QTOF; MS2; CE: 20; R=; [M+H]+

19. Adenosine

[M+H]:268.1040



MS/MS spectrum of Adenosine detected in mouse lung tissue





MS/MS spectrum of Adenosine from MassBank

Adenosine; LC-ESI-QTOF; MS2; [M+H]+; CE: 10eV



20.Inosine

[M+H]:269.0880

MS/MS spectrum of Inosine detected in mouse lung tissue



MS/MS spectrum of Inosine from mzCloud



21.Glutathione

[M+H]:308.0910





MS/MS spectrum of Glutathione from mzCloud



22.Pyroglutamic acid

[M+H]:130.0498

MS/MS spectrum of Pyroglutamic acid detected in mouse lung tissue



MS/MS spectrum of Pyroglutamic acid from mzCloud



23.Histamine

[M+H]:112.0869

MS/MS spectrum of Histamine detected in mouse lung tissue



MS/MS spectrum of Histamine from HMDB



MS/MS spectrum of Histamine from MassBank

Histamine; LC-ESI-QTOF; MS2; HILIC; CE: 10 eV; R=35000; [M+H]+



24.Uric acid

[M-H]:167.0210





MS/MS spectrum of Uric acid from HMDB



25. PGD2

[M+H]:353.2322



MS/MS spectrum of PGD2 detected in mouse lung tissue

MS/MS spectrum of PGD2 from HMDB



26. Adenine

[M+H]:136.0617



MS/MS spectrum of Adenine detected in mouse lung tissue

MS/MS spectrum of Adenine from MassBank

Adenine; LC-ESI-QTOF; MS2; CE:30 V; [M+H]+



Fig S4 MS/MS spectra of different metabolites in serum detected by UPLC-MS/MS.

1.L-Arginine

[M+H]:175.1189

MS/MS spectrum of L-Arginine detected in mouse serum



MS/MS spectrum of L-Arginine from MassBank

L-Arginine; ESI-QTOF; MS2; POSITIVE; [M+H]+; CID; 10 V



2. Kynurenine

[M+H]: 209.0920

MS/MS spectrum of Kynurenine detected in mouse serum







MS/MS spectrum of Kynurenine from MassBank

 Kynurenine; LC-ESI-QTOF; MS2; [M+H]+; CE: 10eV

 Mass Spectrum
 192.0651

 209.0917
 209.0917

3. Glutamate

[M+H]: 148.0604

MS/MS spectrum of Glutamate detected in mouse serum



MS/MS spectrum of Glutamate from HMDB



4. Uric acid

[M+H]: 169.0356

MS/MS spectrum of Uric acid detected in mouse serum



MS/MS spectrum of Uric acid from HMDB



5. LTA4

[M+H]: 319.2267

MS/MS spectrum of LTA4 detected in mouse serum



MS/MS spectrum of LTA4 from HMDB



6. Histidine

[M+H]: 156.0767

MS/MS spectrum of Histidine detected in mouse serum



MS/MS spectrum of Histidine from mz cloud

7. Histamine

[M+H]: 112.0869

MS/MS spectrum of Histamine detected in mouse serum



MS/MS spectrum of Histamine from HMDB

95.0609

112.0875

85.0766

8. Arachidonic acid



MS/MS spectrum of Arachidonic acid detected in mouse serum



MS/MS spectrum of Arachidonic acid from HMDB



MS/MS spectrum of Arachidonic acid from MassBank

Arachidonic acid; LC-ESI-QTOF; MS2; CE:20 eV; [M-H]-



9. Uridine

[M-H]: 243.0622

MS/MS spectrum of Uridine detected in mouse serum



MS/MS spectrum of Uridine from mz cloud

MS/MS spectrum of Uridine from MassBank

onume,	LC-ESI-QIOF, MSZ, CE. ZU,	к—, [IVI-	- I-
Mass Spectrum	110.0256		
	2	00.0566	243.0602

Uridine; LC-ESI-QTOF; MS2; CE: 20; R=; [M-H]-

10. Xanthine

[M+H]: 153.0407



MS/MS spectrum of Xanthine detected in mouse serum

MS/MS spectrum of Xanthine standard



MS/MS spectrum of Xanthine from MassBank

Xanthine; LC-ESI-QTOF; MS2; CE: 20; R=; [M+H]+

Mass Spectrum		110.03	849	
		110.00	7-5	153.0400
	82.0394			

11. Tryptophan

[M+H]: 205.0971

MS/MS spectrum of Tryptophan detected in mouse serum



MS/MS spectrum of Tryptophan from mz cloud

MS/MS spectrum of Tryptophan from MassBank

L-Tryptophan; LC-ESI-QTOF; MS2; CE 10 ev; [M+H]+

12. 5-HPETE

[M+H]: 337.2373

MS/MS spectrum of 5-HPETE detected in mouse serum

MS/MS spectrum of 5-HPETE from HMDB

319.2268

301.2162 337.2373

119.0855

13. α-Linolenic acid

[M-H]: 277.2173

MS/MS spectrum of α -Linolenic acid detected in mouse serum

MS/MS spectrum of α -Linolenic acid from HMDB

14. Linoleic acid

MS/MS spectrum of linoleic acid standard

15. Valine

[M+H]: 118.0863

MS/MS spectrum of Valine detected in mouse serum

MS/MS spectrum of Valine from HMDB

