SUPPLEMENTARY MATERIALS

A urinary metabolomics study of the metabolic dysfunction and the regulation effect of citalopram in the rats exposed to chronic unpredictable mild stress

Xinyu Yu[a#], Jia Luo[b#], Lijun Chen[a], Chengxiang Zhang[b], Rutan Zhang[a], Qi Hu[b], Shanlei Qiao[b✉], Lei Li[a✉]

[a]*Department of Hygiene Analysis and Detection, School of Public Health, Nanjing Medical University, Nanjing, Jiangsu 211166, P. R. China*
[b]*The Key Laboratory of Modern Toxicology, Ministry of Education, School of Public Health, Nanjing Medical University, Nanjing 211166, Jiangsu, P.R. China.*

✉*Corresponding authors:*
Lei Li, Department of hygiene analysis and detection, School of Public Health, Nanjing Medical University, 101 Longmian Avenue, Nanjing 211166, P. R. China
Tel: +86-25-8686-8404; Fax: +86-25-8686-8499; E-mail: drleili@hotmail.com
Shanlei Qiao, The Key Laboratory of Modern Toxicology, Ministry of Education, School of Public Health, Nanjing Medical University, Nanjing 211166, Jiangsu, P.R. China.
Tel: +86-25-8686-8402; Fax: +86-25-8686-8499; E-mail: alexqiao@139.com

S1. Supporting Results

This section involves the comparison of MS/MS spectra with authentic standards, the retention time shift of each compound, and the putative identification of compounds without authentic standards.

Glycerol

Figure Legends

S-Fig.1 (a) MS/MS spectra of glycerol in urine sample. (b) MS/MS spectra of authentic standard

Fig.1a

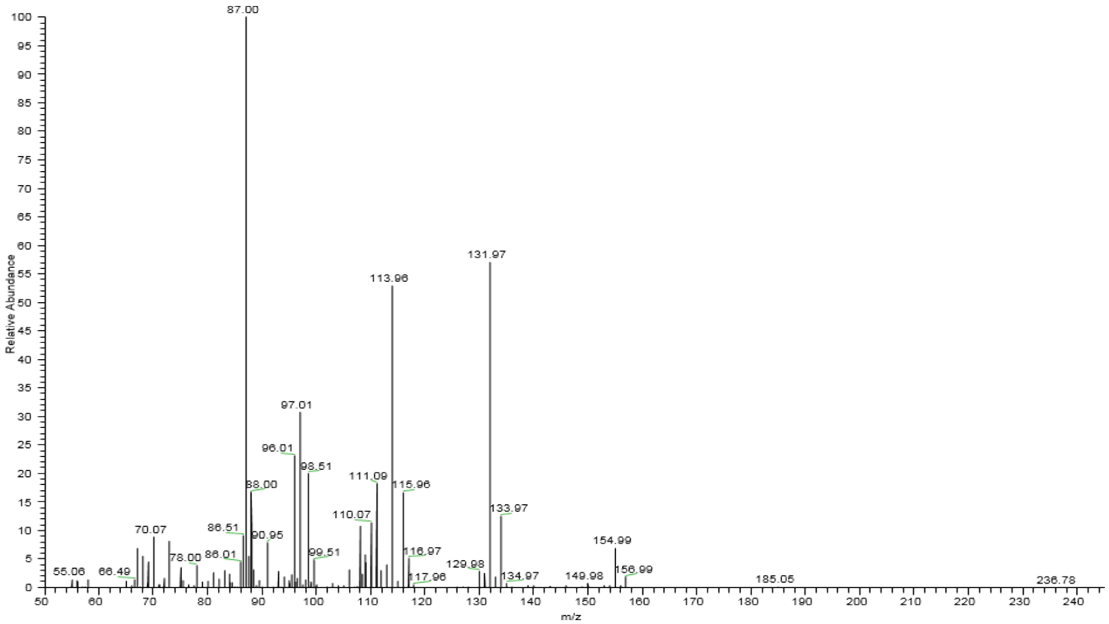
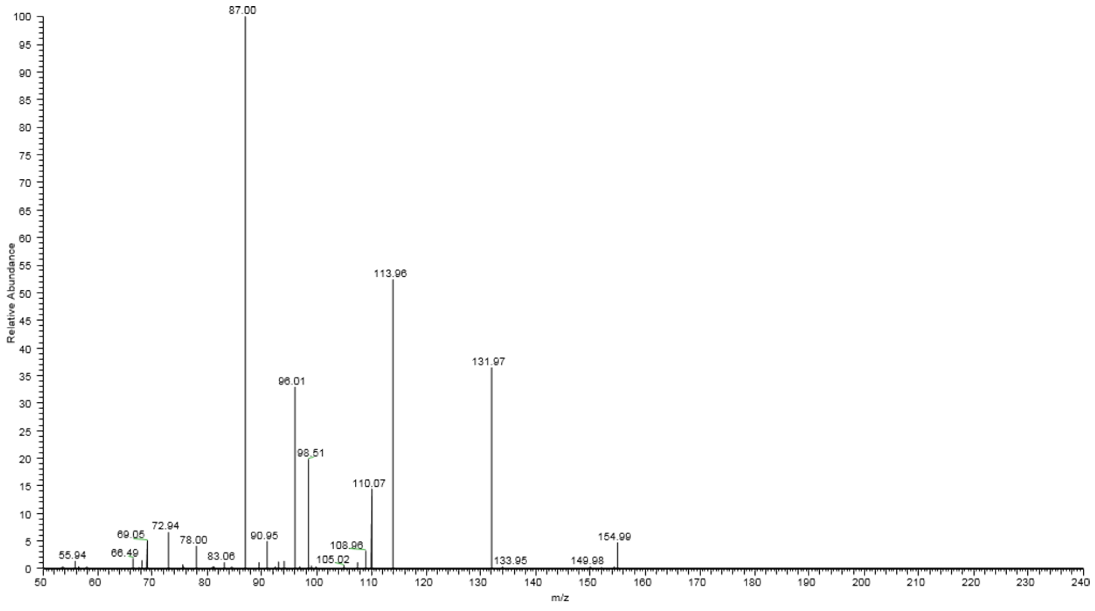


Fig.1b



Succinic acid

Figure Legends

S-Fig.2 (a) MS/MS spectra of succinic acid in urine sample. (b) MS/MS spectra of authentic standard

Fig.2a

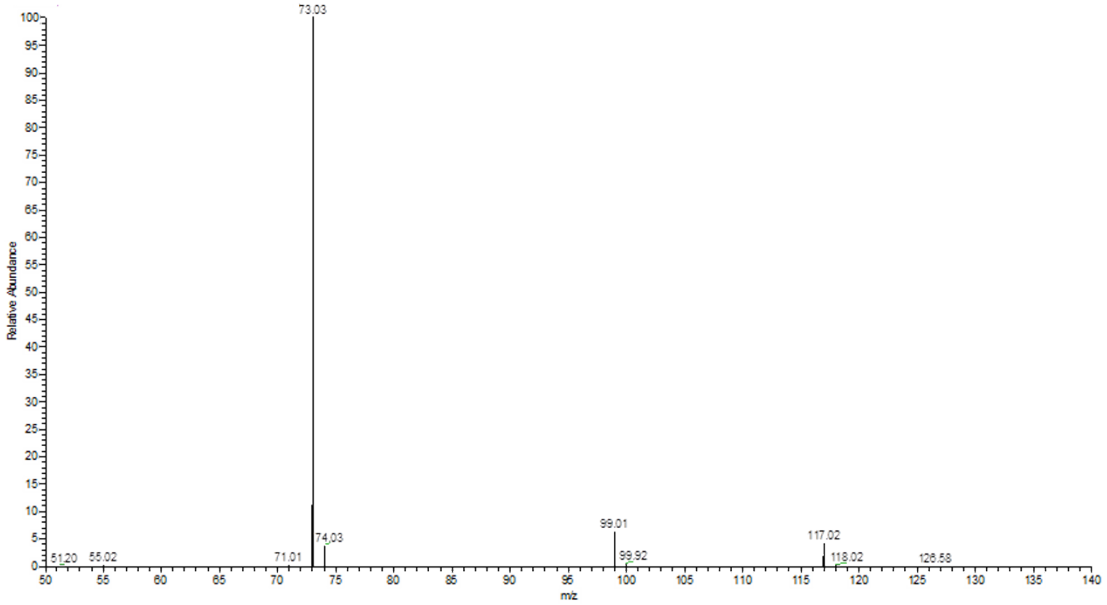
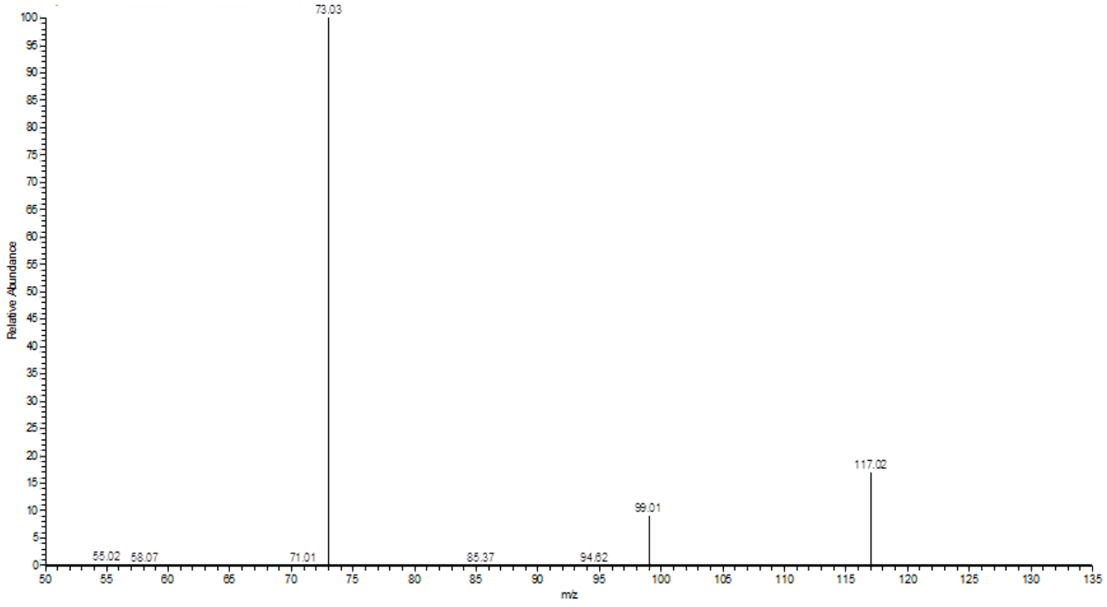


Fig.2b



Creatine

Figure Legends

S-Fig.3 (a) MS/MS spectra of creatine in urine sample. (b) MS/MS spectra of authentic standard

Fig.3a

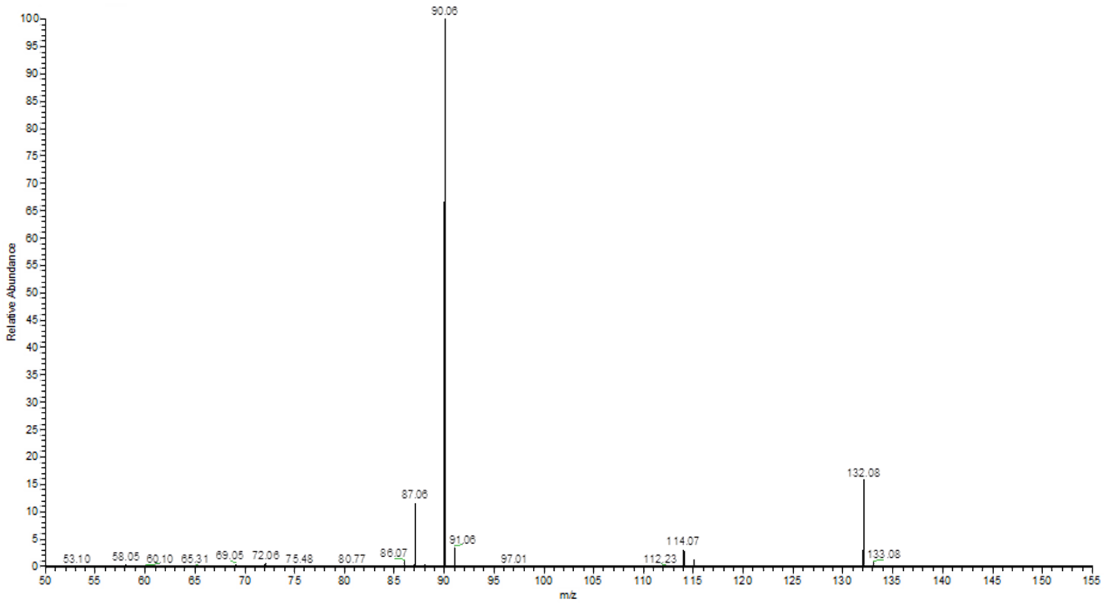
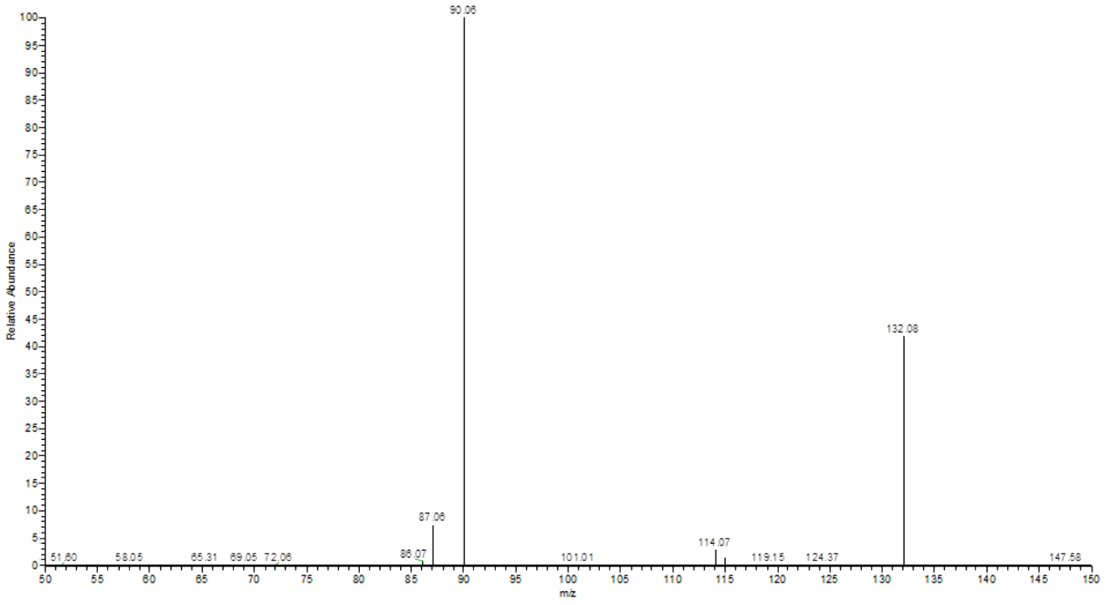


Fig.3b



Quinolinic acid

Figure Legends

S-Fig.4 (a) MS/MS spectra of quinolinic acid in urine sample. (b) MS/MS spectra of authentic standard

Fig.4a

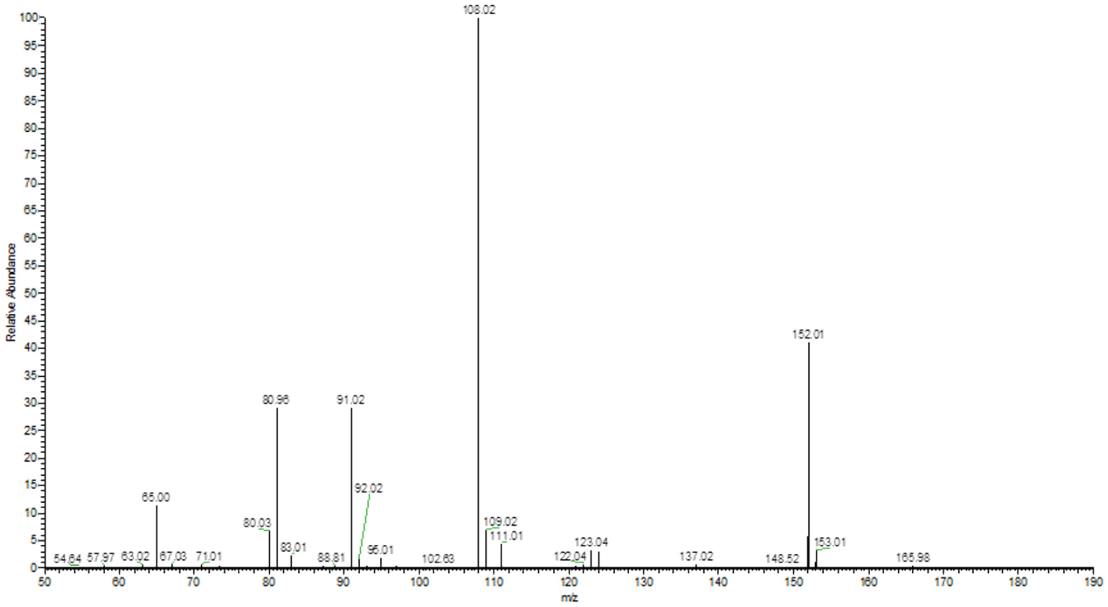
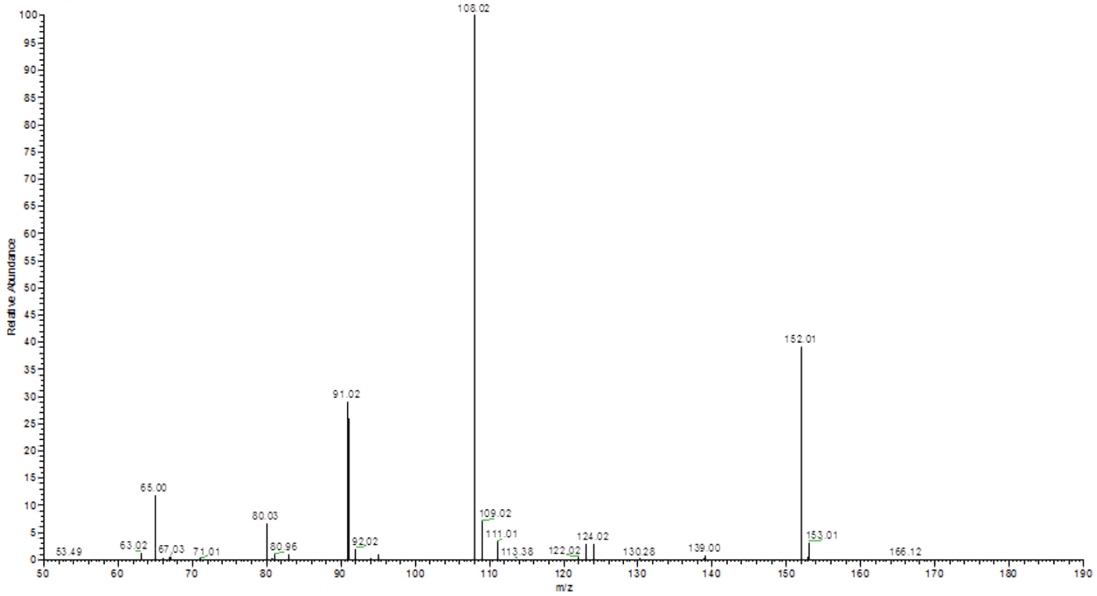


Fig.4b



L-Phenylalanine

Figure Legends

S-Fig.5 (a) MS/MS spectra of L-phenylalanine in urine sample. (b) MS/MS spectra of authentic standard

Fig.5a

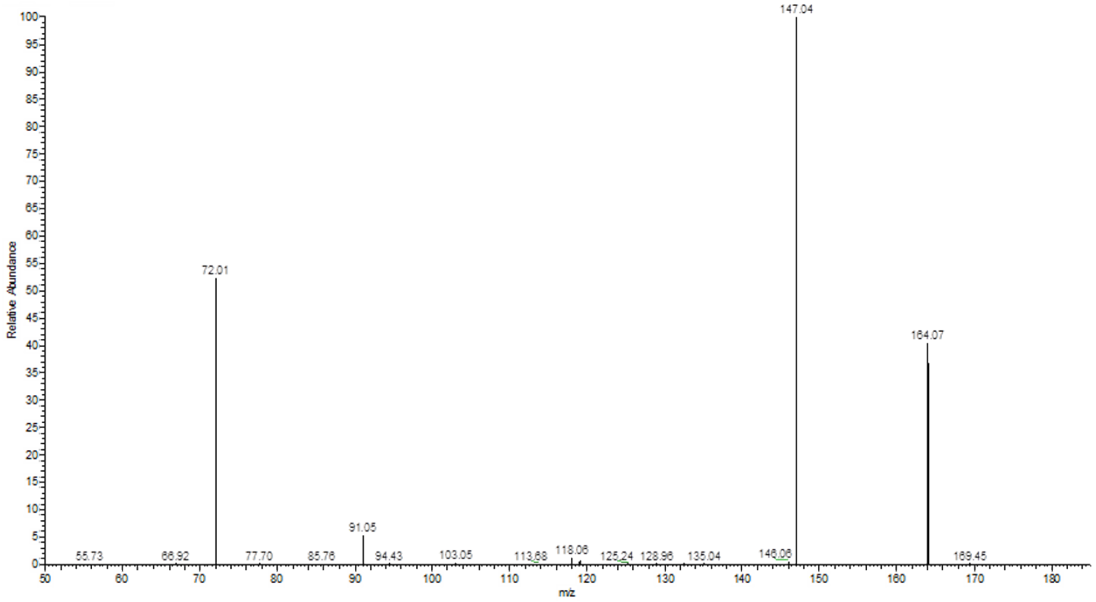
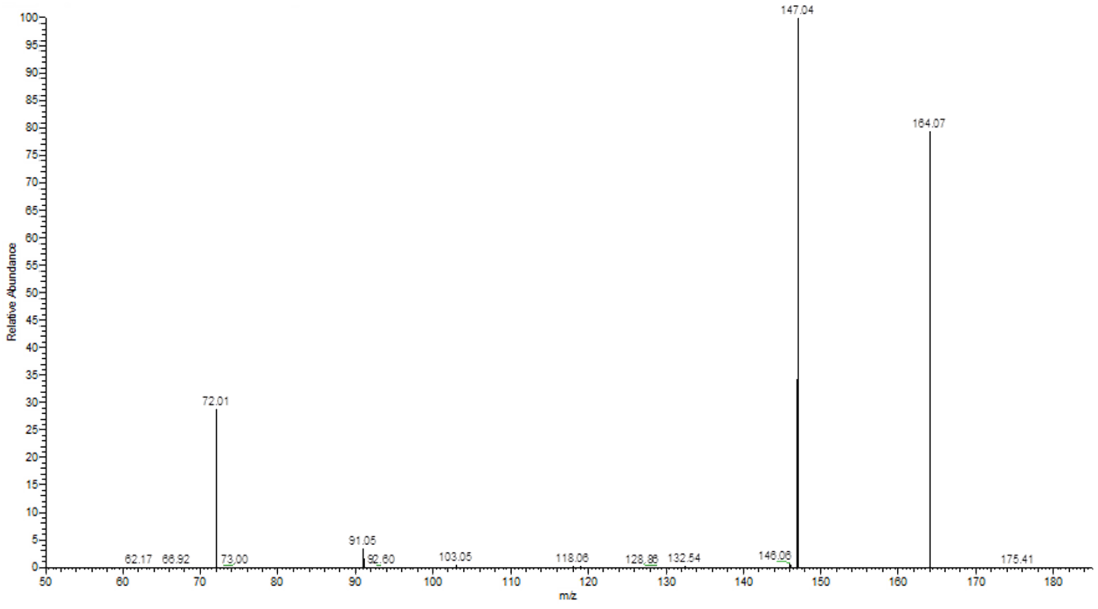


Fig.5b



Gamma-Aminobutyric acid

Figure Legends

S-Fig.6 (a) MS/MS spectra of Gamma-aminobutyric acid in urine sample. (b) MS/MS spectra of authentic standard

Fig.6a

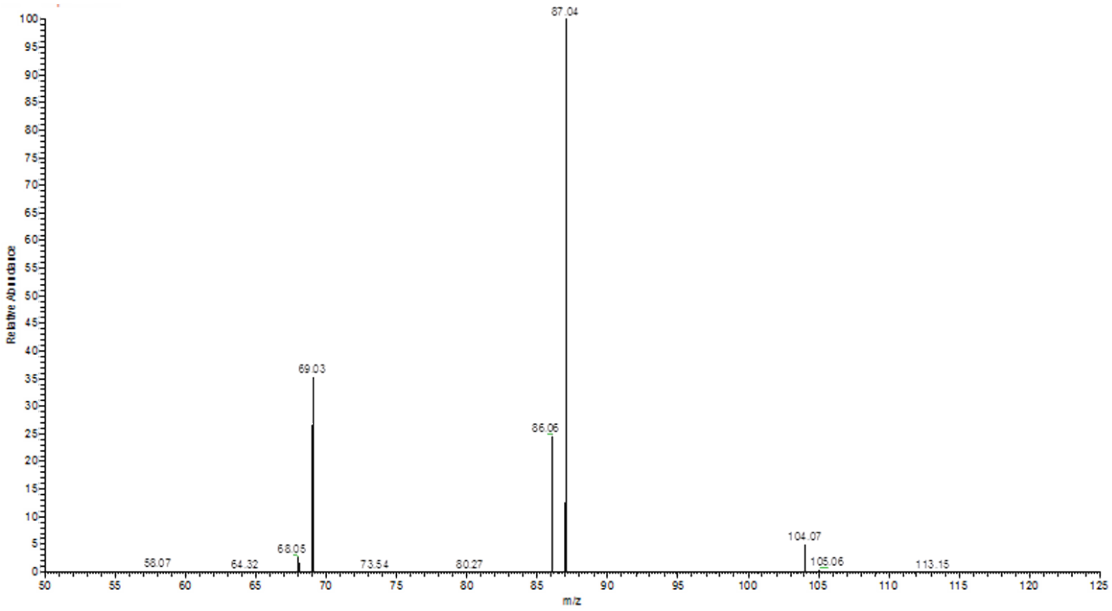
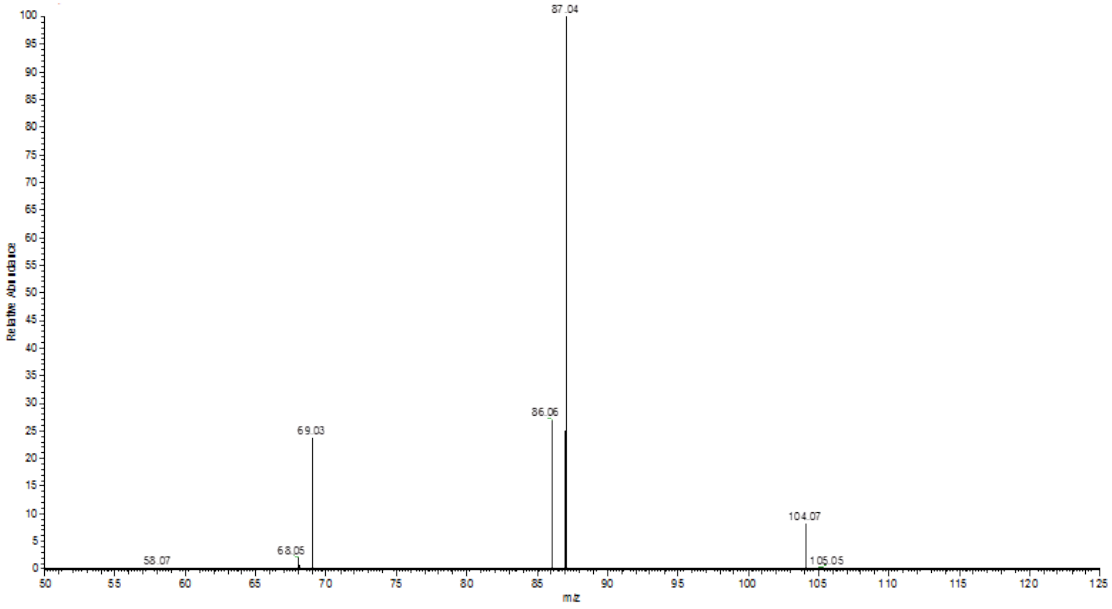


Fig.6b



Dopamine

Figure Legends

S-Fig.7 (a) MS/MS spectra of Dopamine in urine sample. (b) MS/MS spectra of authentic standard

Fig.7a

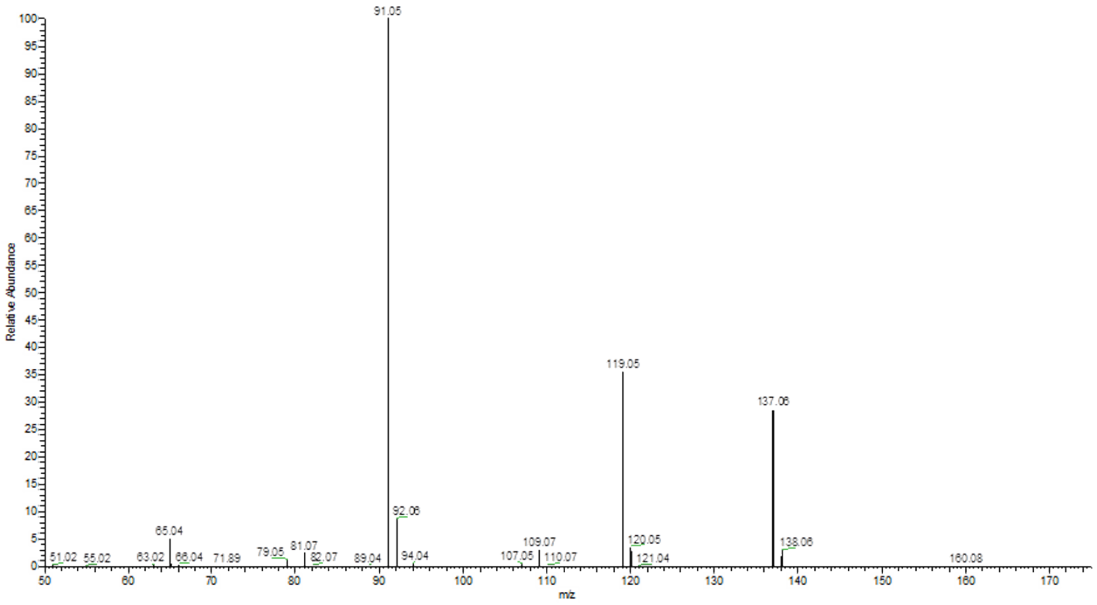
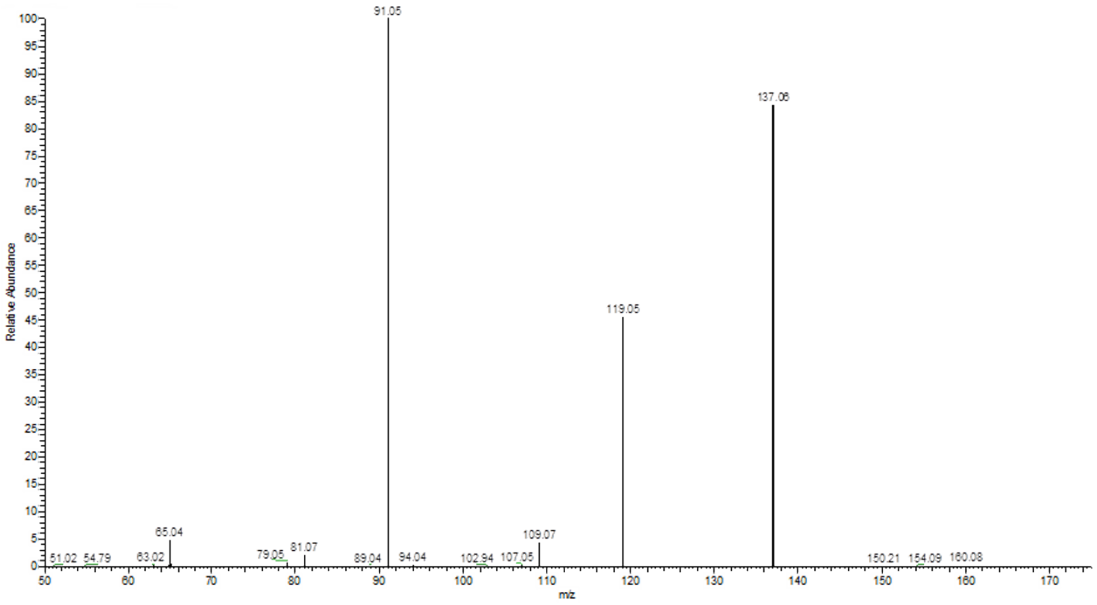


Fig.7b



L-Tryptophan

Figure Legends

S-Fig.8 (a) MS/MS spectra of L-tryptophan in urine sample. (b) MS/MS spectra of authentic standard

Fig.8a

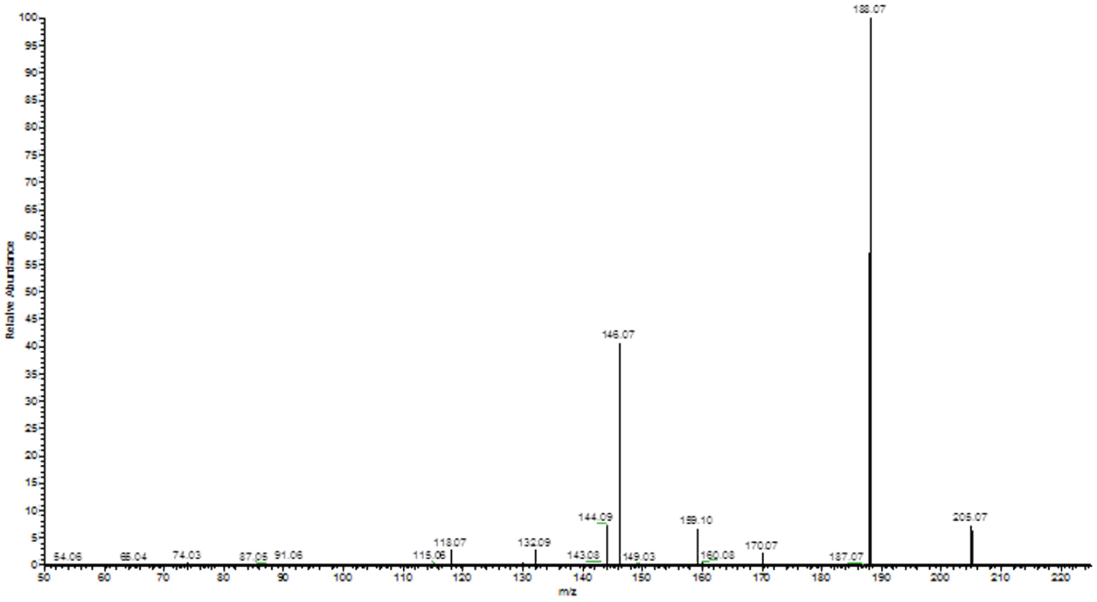
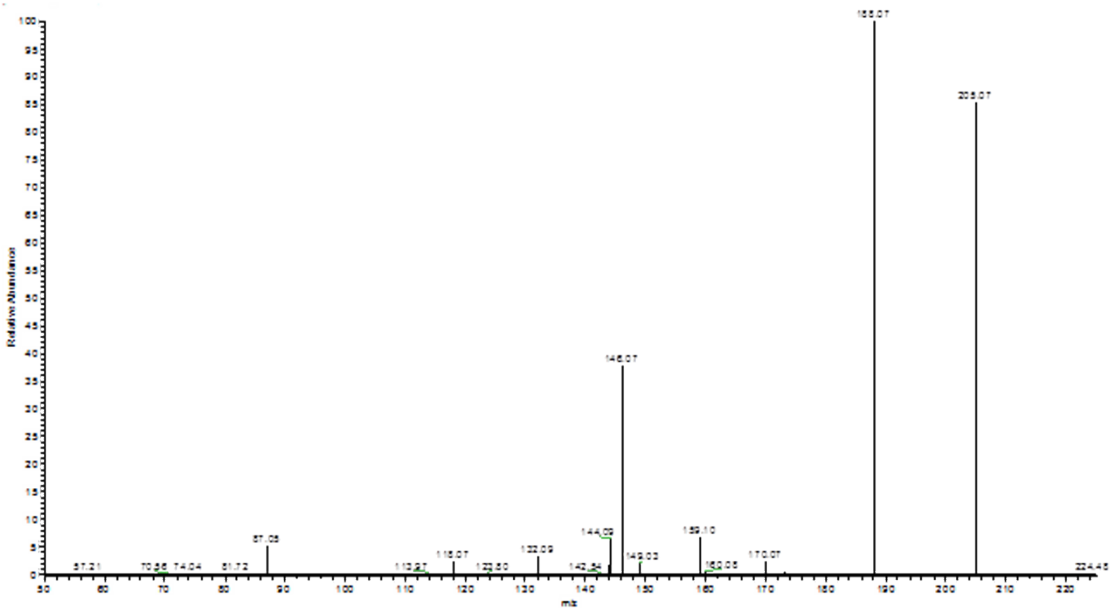


Fig.8b



L-Isoleucine

Figure Legends

S-Fig.9 (a) MS/MS spectra of L-isoleucine in urine sample. (b) MS/MS spectra of authentic standard

Fig.9a

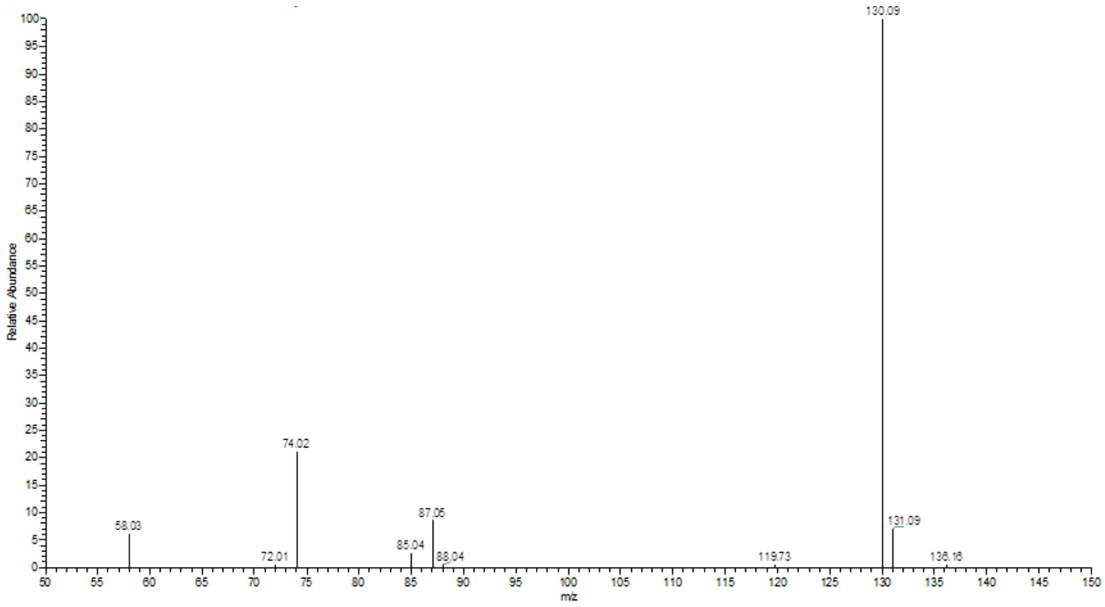
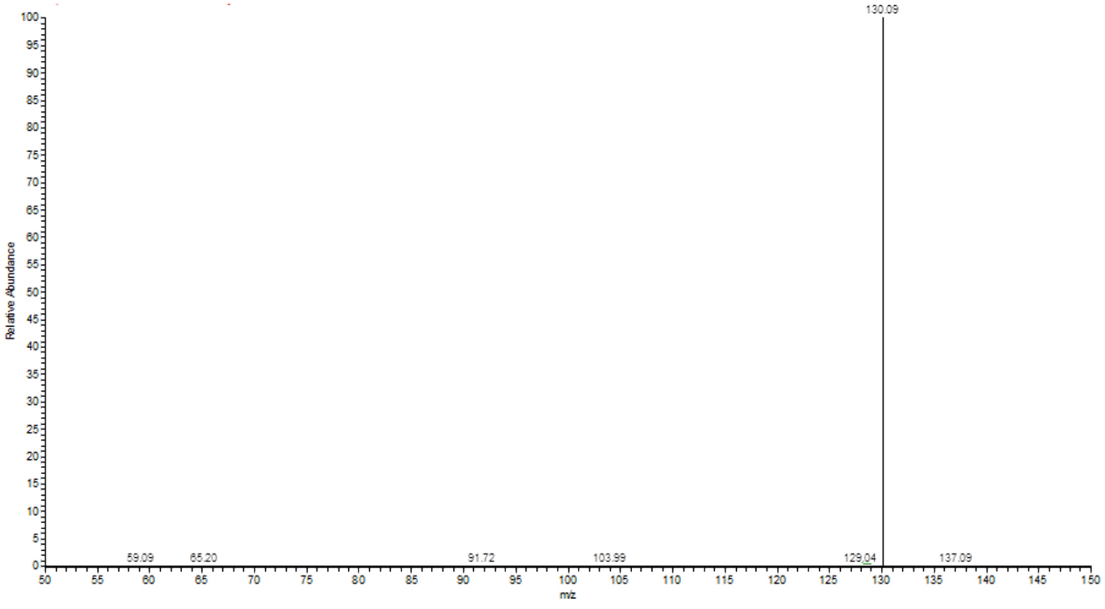


Fig.9b



L-Serine

Figure Legends

S-Fig.10 (a) MS/MS spectra of L-serine in urine sample. (b) MS/MS spectra of authentic standard

Fig.10a

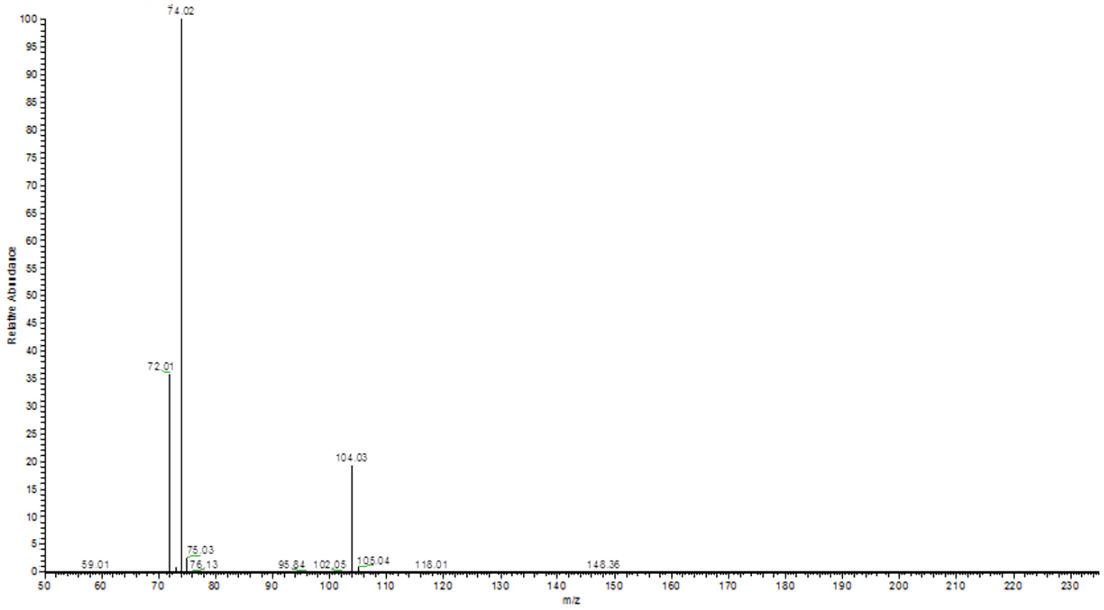
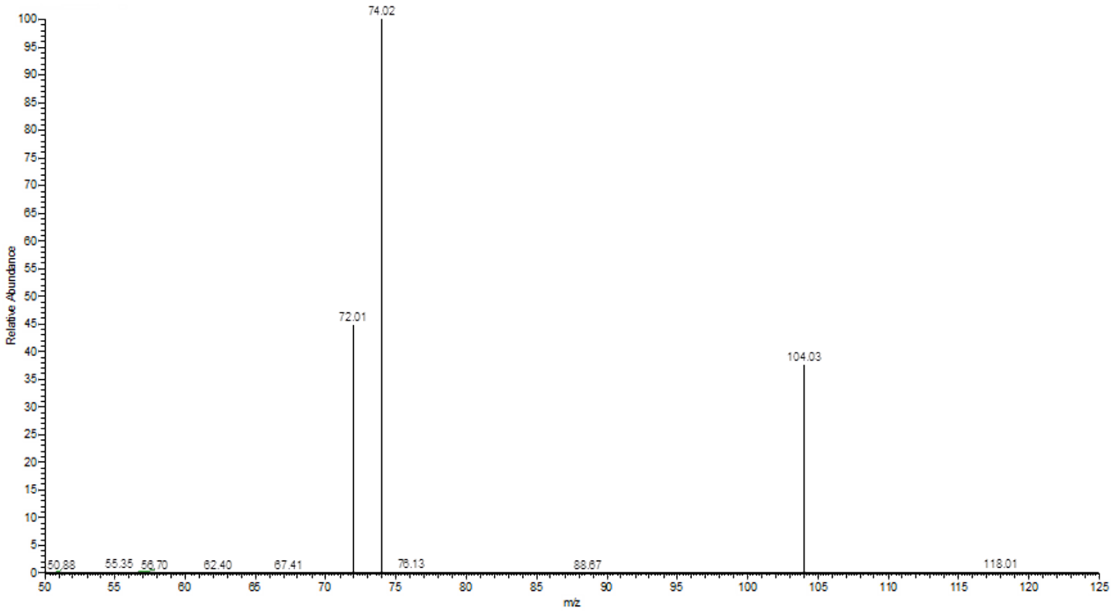


Fig.10b



Hypoxanthine

Figure Legends

S-Fig.11 (a) MS/MS spectra of hypoxanthine in urine sample. (b) MS/MS spectra of authentic standard

Fig.11a

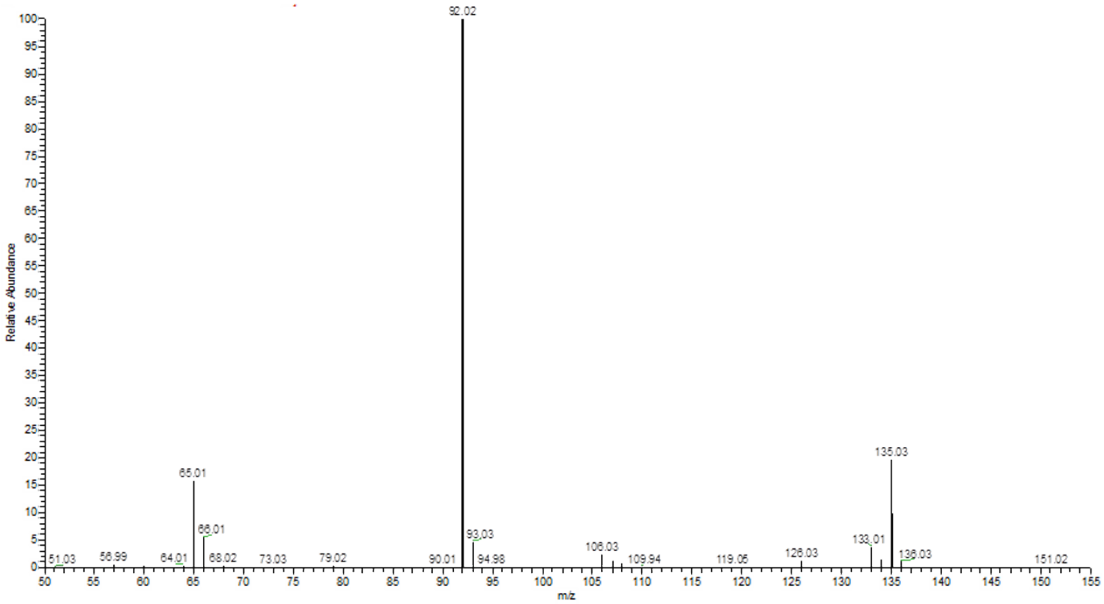
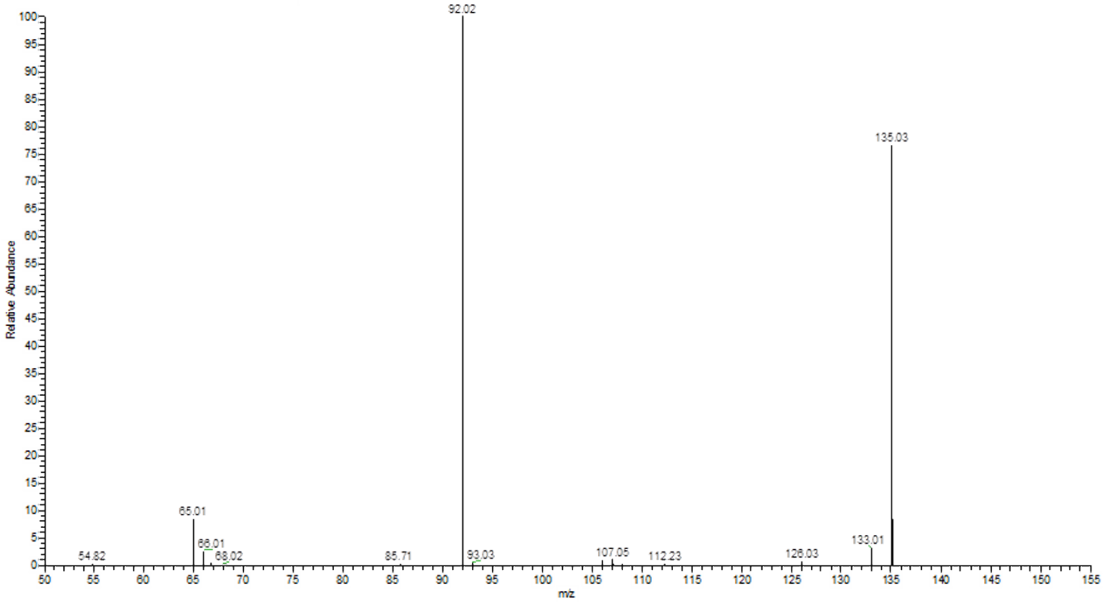


Fig.11b



Pyruvic acid

Figure Legends

S-Fig.12 (a) MS/MS spectra of pyruvic acid in urine sample. (b) MS/MS spectra of authentic standard

Fig.12a

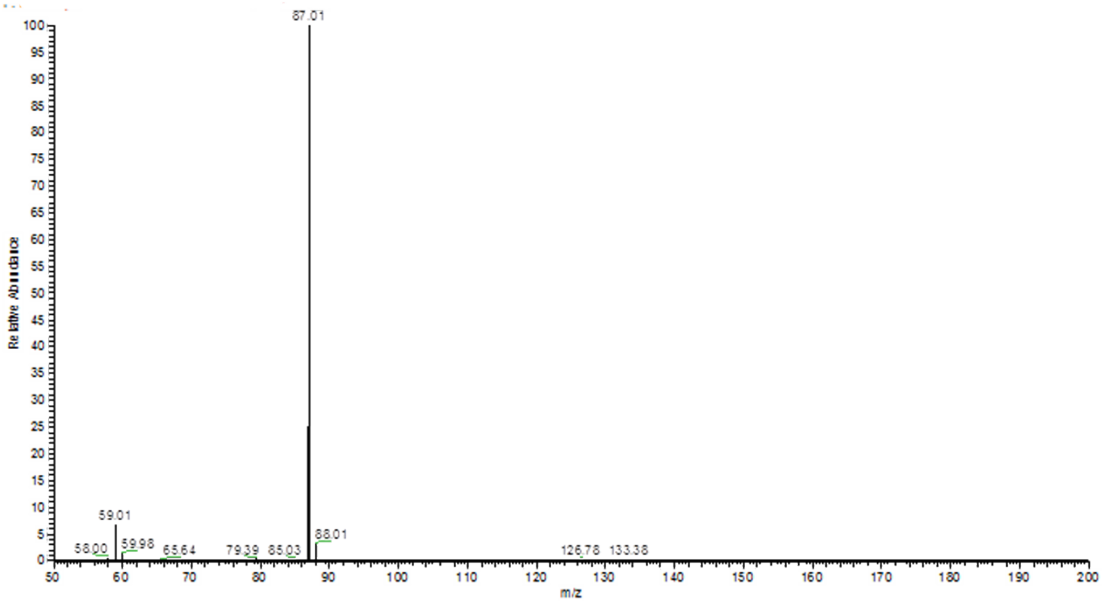
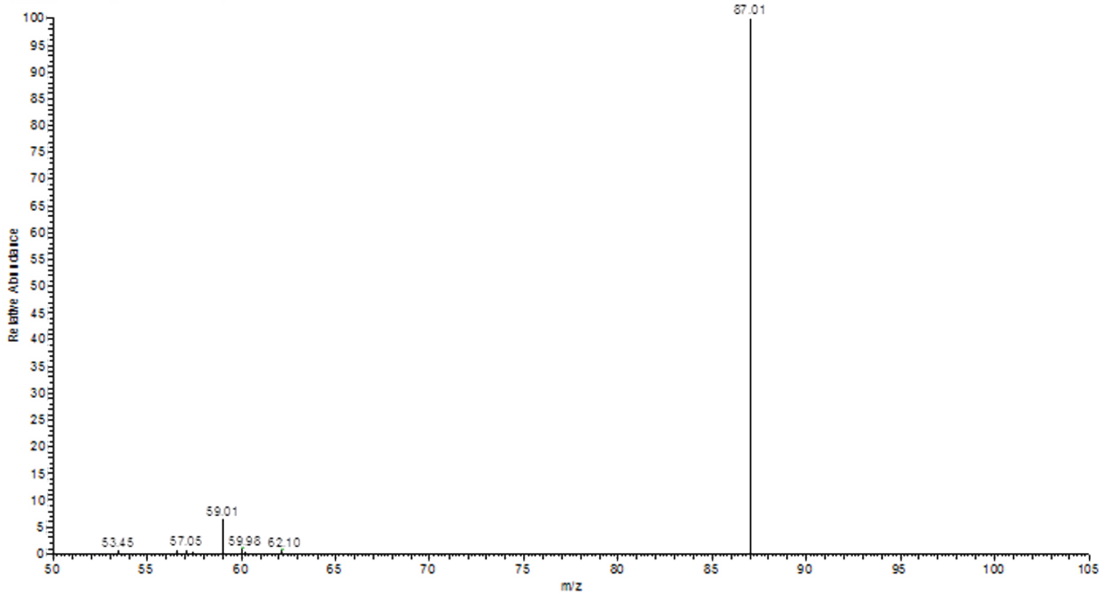


Fig.12b



Indoleacetic acid

Figure Legends

S-Fig.13 (a) MS/MS spectra of indoleacetic acid in urine sample. (b) MS/MS spectra of authentic standard

Fig.13a

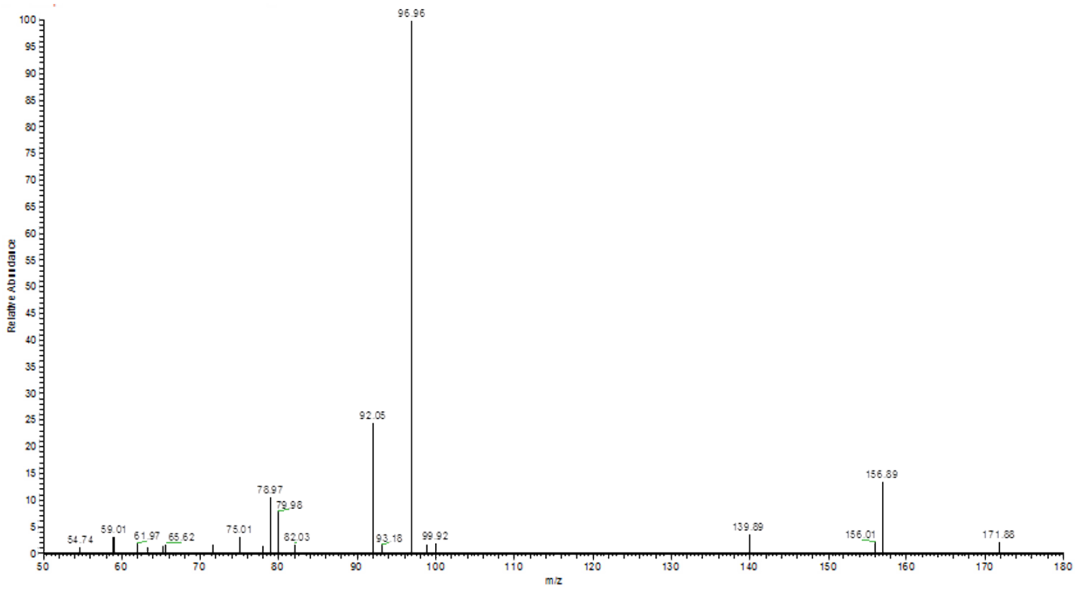
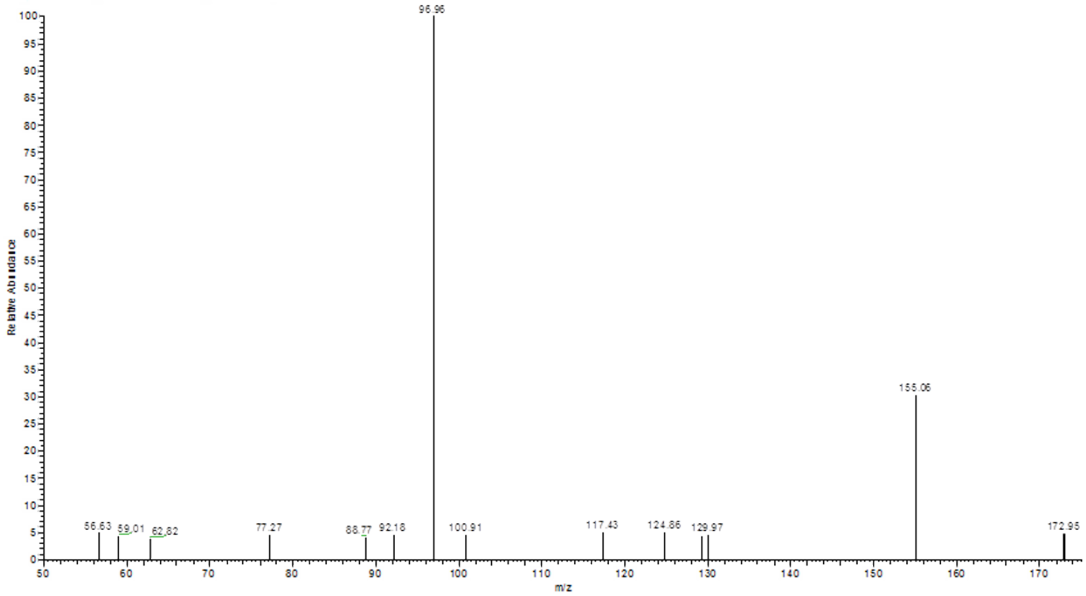


Fig.13b



Citric acid

Figure Legends

S-Fig.14 (a) MS/MS spectra of citric acid in urine sample. (b) MS/MS spectra of authentic standard

Fig.14a

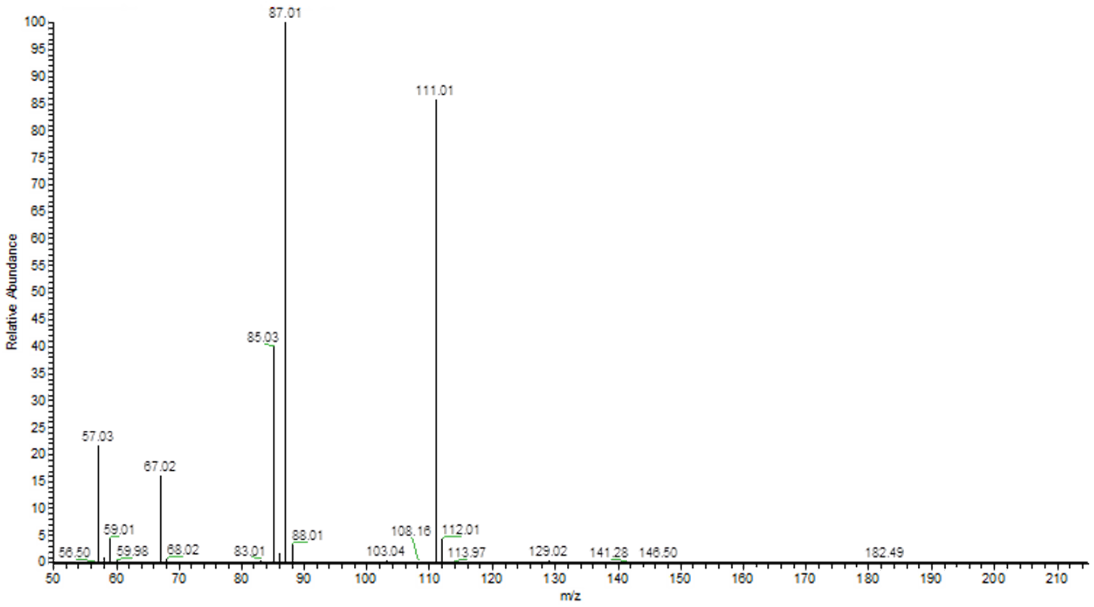
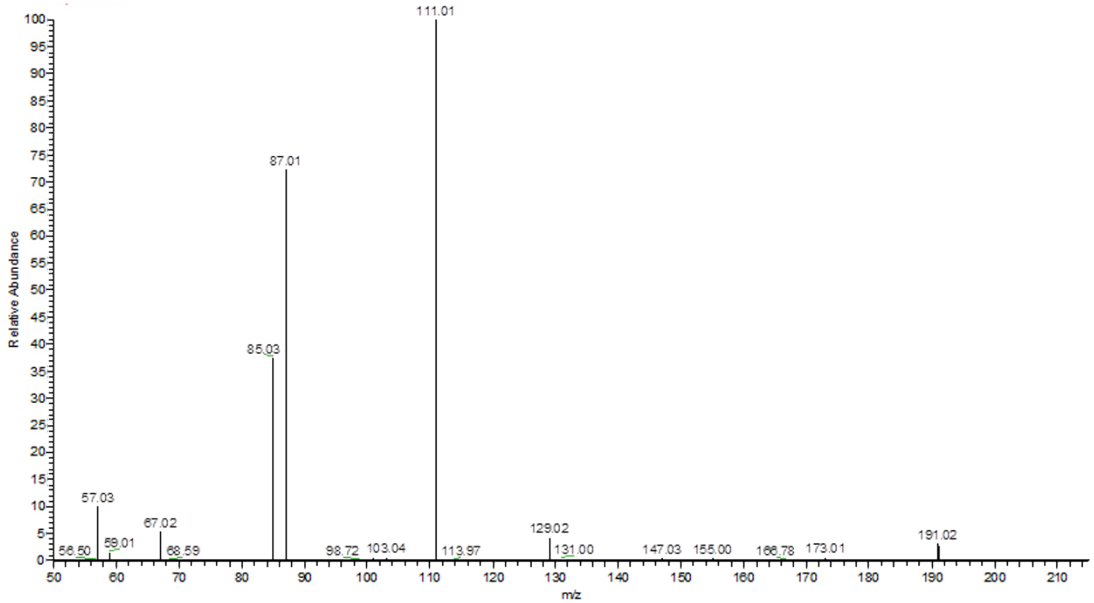


Fig.14b



L-Dopa

Figure Legends

S-Fig.15 (a) MS/MS spectra of L-dopa in urine sample. (b) MS/MS spectra of authentic standard

Fig.15a

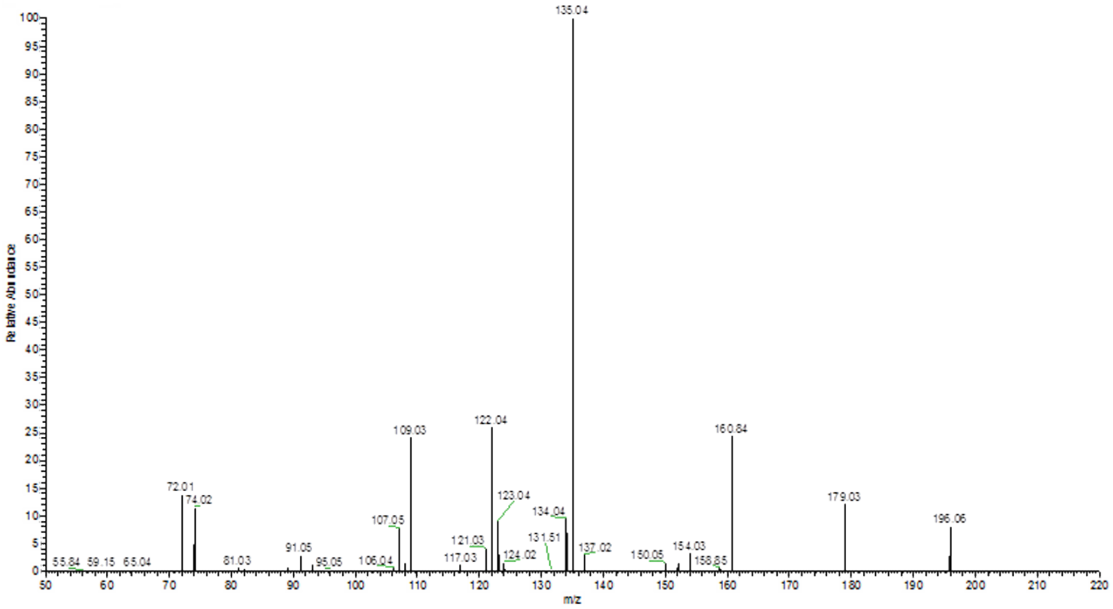
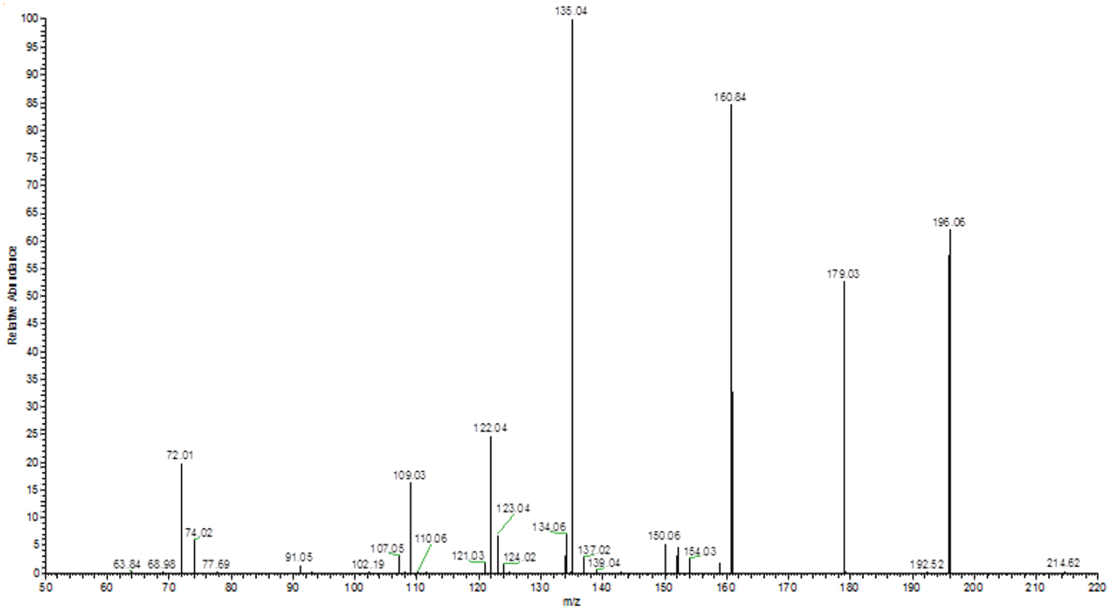


Fig.15b



Glycine

Figure Legends

S-Fig.16 (a) MS/MS spectra of glycine in urine sample. (b) MS/MS spectra of authentic standard

Fig.16a

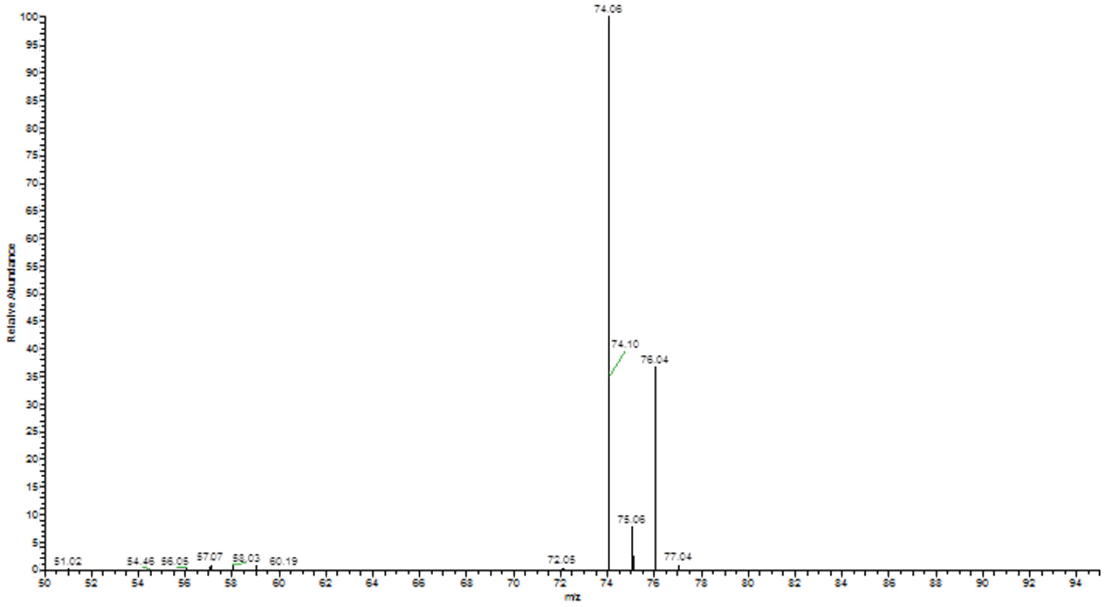
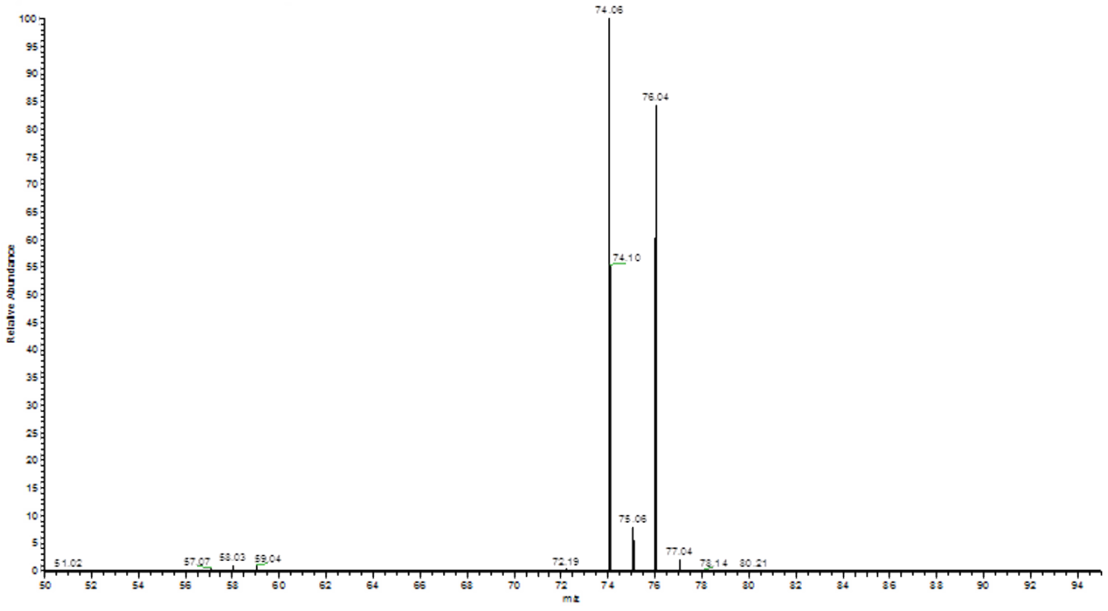


Fig.16b



Supporting table.1. Retention time shift of each compound

No	Metabolite	t_R (min)	Shift(min)
1	Glycerol	1.34	0.03
2	Succinic acid	0.66	0.02
3	Creatine	5.49	0.12
4	Quinolinic acid	0.99	0.03
5	L-Phenylalanine	6.49	0.16
6	Kynurenic acid	4.87	0.08
7	Gamma-Aminobutyric acid	7.30	0.19
8	L-Kynurenine	5.72	0.11
9	Dopamine	5.25	0.10
10	L-Tryptophan	4.89	0.08
11	L-Isoleucine	1.24	0.03
12	L-Serine	1.11	0.03
13	Hypoxanthine	1.34	0.03
14	5-hydroxyindoleacetic acid	3.72	0.05
15	N-Acetyl-L-aspartic acid	4.36	0.07
16	Pyruvic acid	0.70	0.02
17	Phenylacetylglycine	5.53	0.10
18	Indoleacetic acid	6.74	0.13
19	Citric acid	6.55	0.12
20	L-Dopa	5.35	0.10
21	Glycine	3.22	0.05

Putative identification of compounds without authentic standards

For these compounds, the databases of HMDB (http://www.hmdb.ca/) is searched for candidates with molecular weight similar with that found in our experiment at the tolerance of 5ppm, and choose the HMDB ID before 5000 which means it is relatively common in our body.

Metabolite	t_R (min)	Measured Molecular Weight	HMDB matching	Monoisotopic Molecular Weight	Diff (ppm)
4,6-Dihydroxyquinoline	6.10	161.0472132	HMDB04077	161.047678473	2.89
Indole-3-carboxylic acid	5.47	161.0470437	HMDB03320	161.047678473	3.94
Indoxyl sulfate	2.72	213.0090460	HMDB00682	213.009578407	2.50
Phenylpyruvic acid	0.74	164.0469798	HMDB00205	164.047344122	2.22
Xanthurenic acid	5.62	205.0369086	HMDB00881	205.037507717	2.92