

Table S1 The main compounds of FTE using UPLC-QTOF-MS/MS

No.	ID	Name	mz	RT(s)	Exact mass	Formula	KEGG	Type	Library	Identify pvalue	Superpathway	Class
1	M257T455	(2S)-Liquiritigenin	257.1859716	455.313	256.0736	C15H12O4	C09762	[M+H] ⁺	BioDeepDB	0.004844582	Lipid	Flavonoids
2	M301T551	Hesperetin	301.2019364	550.779	302.079	C16H14O6	C01709	[M-H] ⁻	BioDeepDB	0.197456826	Lipid	Flavonoids
3	M287T761	Luteolin	287.1745333	761.397	286.0477	C15H10O6	C01514	[M+H] ⁺	BioDeepDB	0.079155907	Lipid	Flavonoids
4	M87T89	(R)-3-Hydroxybutyric acid	87.0447555	89.1543	104.0473	C4H8O3	C01089	[M+H-H2O] ⁺	BioDeepDB	2.10705E-06	Carbohydrate	Hydroxy acids and derivatives
5	M215T665	12-Hydroxydodecanoic acid	215.0128231	664.796	216.1725	C12H24O3	C08317	[M-H] ⁻	BioDeepDB	2.81988E-13	Lipid	Hydroxy acids and derivatives
6	M177T284	Gulonic acid	177.0392703	284.239	196.0583	C6H12O7	C00800	[M-H2O-H] ⁻	GNPS	0.000100522	Carbohydrate	Hydroxy acids and derivatives
7	M133T90	Malate	133.0146619	89.8838	134.0215	C4H6O5	C00711	[M-H] ⁻	mzCloud	0.000407619	Unknow	Hydroxy acids and derivatives
8	M174T123	1H-Indole-3-acetamide	174.0771066	123.223	174.0793	C10H10N2O	C02693	[M] ⁻	BioDeepDB	0.768254275	Amino acid	Indoles and derivatives
9	M146T582	1H-Indole-3-carboxaldehyde	146.0607806	581.823	145.0528	C9H7NO	C08493	[M+H] ⁺	MoNA	4.0806E-06	Unknow	Indoles and derivatives
10	M157T47	3-Indoleacetoneitrile	157.0858269	46.8638	156.0687	C10H8N2	C02938	[M+H] ⁺	BioDeepDB	8.02692E-16	Amino acid	Indoles and derivatives
11	M192T395	5-Hydroxyindoleacetate	192.0663177	394.863	191.0582	C10H9NO3	C05635	[M+H] ⁺	mzCloud	5.17992E-05	Amino acid	Indoles and derivatives
12	M191T792	5-Hydroxyindoleacetic acid	191.1079931	792.409	191.0582	C10H9NO3	C05635	[M] ⁻	BioDeepDB	1.43474E-09	Amino acid	Indoles and derivatives
13	M204T458	5-Methoxyindoleacetate	204.0669419	457.612	205.0739	C11H11NO3	C05660	[M-H] ⁻	BioDeepDB	4.9298E-06	Amino acid	Indoles and derivatives
14	M248T478	6-Hydroxymelatonin	248.1128988	478.2	248.1161	C13H16N2O	C05643	[M] ⁺	BioDeepDB	5.94458E-08	Amino acid	Indoles and derivatives
15	M169T461	Beta-Carboline	169.0761002	460.714	168.0687	C11H8N2	C20157	[M+H] ⁺	MoNA	1.90078E-08	ofactors and Vitamin	Indoles and derivatives
16	M189T494	Dimethyltryptamine	189.1382226	493.628	188.1313	C12H16N2	C08302	[M+H] ⁺	BioDeepDB	0.144682319	Unknow	Indoles and derivatives
17	M175T386	Gramine	175.1228275	386.224	174.1157	C11H14N2	C08304	[M+H] ⁺	MoNA	0.280568682	Amino acid	Indoles and derivatives
18	M117T113	Indole	117.0547885	112.901	117.0578	C8H7N	C00463	[M] ⁺	BioDeepDB	0.00261501	Amino acid	Indoles and derivatives
19	M176T599	Indole-3-acetate	176.0703419	599.248	175.0633	C10H9NO2	C00954	[M+H] ⁺	mzCloud	6.75114E-23	Amino acid	Indoles and derivatives
20	M162T564	Indole-3-carboxylic acid	162.054805	563.736	161.0477	C9H7NO2	C19837	[M+H] ⁺	MoNA	7.85205E-11	Amino acid	Indoles and derivatives
21	M203T362	Indolebutyric acid	203.0931876	362.07	203.0946	C12H13NO2	C11284	[M] ⁻	mzCloud	0.248417782	Unknow	Indoles and derivatives
22	M188T473	Indolelactic acid	188.0705759	472.689	205.0739	C11H11NO3	C02043	[M+H-H2O] ⁺	MoNA	0.144682311	Amino acid	Indoles and derivatives
23	M191T435	N-Methylserotonin	191.1176524	435.143	190.1106	C11H14N2O	C06212	[M+H] ⁺	BioDeepDB	5.78073E-06	Amino acid	Indoles and derivatives
24	M249T527	Pindolol	249.1592902	526.803	248.1525	C14H20N2O	C07445	[M+H] ⁺	BioDeepDB	1.87362E-06	Unknow	Indoles and derivatives
25	M161T428	Tryptamine	161.1083364	427.728	160.1	C10H12N2	C00398	[M+H] ⁺	BioDeepDB	1.24815E-16	Amino acid	Indoles and derivatives
26	M144T427_2	Tryptophanol	144.0798299	426.665	161.0841	C10H11NO	C00955	[M+H-H2O] ⁺	BioDeepDB	0.000135609	Amino acid	Indoles and derivatives
27	M283T689	Biochanin A	283.0605701	688.739	284.0685	C16H12O5	C00814	[M-H] ⁻	BioDeepDB	1.10818E-10	Lipid	Isoflavonoids
28	M267T734	Formononetin	267.0680944	734.417	268.0736	C16H12O4	C00858	[M-H] ⁻	BioDeepDB	8.23517E-13	Lipid	Isoflavonoids
29	M271T655	Genistein	271.1795415	655.327	270.0528	C15H10O5	C06563	[M+H] ⁺	BioDeepDB	3.91102E-08	Lipid	Isoflavonoids
30	M337T116_2	Psoralidin	337.1120992	115.989	336.0998	C20H16O5	C10523	[M+H] ⁺	mzCloud	8.73379E-05	Lipid	Isoflavonoids
31	M165T515_1	3-Methoxy-4-hydroxyphenylglycolaldehyde	165.0537304	515.424	182.0579	C9H10O4	C05583	[M+H-H2O] ⁺	MetaDNA	0.003330742	Amino acid	Phenols
32	M167T358	3,4-Dihydroxyphenylacetate	167.0351799	358.172	168.0423	C8H8O4	C01161	[M-H] ⁻	mzCloud	0.01108441	Amino acid	Phenols
33	M137T646	4-Hydroxyphenylethanol	137.0609223	646.492	138.0681	C8H10O2	C06044	[M-H] ⁻	mzCloud	0.000271927	Amino acid	Phenols
34	M125T468	4-Methylcatechol	125.0603275	468.229	124.0524	C7H8O2	C06730	[M+H] ⁺	BioDeepDB	3.92574E-07	Xenobiotics	Phenols
35	M302T449	Dobutamine	302.1727473	448.965	301.1678	C18H23NO3	C06967	[M+H] ⁺	mzCloud	2.64925E-05	Unknow	Phenols
36	M154T164	Dopamine	154.0864564	164.467	153.079	C8H11NO2	C03758	[M+H] ⁺	BioDeepDB	3.03341E-05	Amino acid	Phenols
37	M166T317	Epinephrine	166.0862558	317.016	183.0895	C9H13NO3	C00788	[M+H-H2O] ⁺	MoNA	3.98495E-05	Amino acid	Phenols
38	M183T39	Homovanillic acid	183.0647637	39.0339	182.0579	C9H10O4	C05582	[M+H] ⁺	BioDeepDB	0.001805929	Amino acid	Phenols
39	M111T301_1	Hydroquinone	111.0439957	301.352	110.0368	C6H6O2	C00530	[M+H] ⁺	MoNA	2.37762E-10	Xenobiotics	Phenols
40	M240T567	Isoetharine	240.1587777	567.165	239.1521	C13H21NO3	C07053	[M+H] ⁺	BioDeepDB	0.050040993	Unknow	Phenols
41	M109T701	m-Cresol	109.1006382	700.813	108.0575	C7H8O	C01467	[M+H] ⁺	BioDeepDB	8.23957E-05	Xenobiotics	Phenols
42	M152T141	Norepinephrine	152.0693286	140.706	169.0739	C8H11NO3	C00547	[M+H-H2O] ⁺	BioDeepDB	4.20074E-06	Amino acid	Phenols

43	M212T556	Orciprenaline	212.1280464	555.576	211.1208	C11H17NO3	C07144	[M+H] ⁺	BioDeepDB	9.02016E-09	Unknow	Phenols
44	M150T383_2	p-Synephrine	150.0913223	382.911	167.0946	C9H13NO2	C04548	[M+H-H2O] ⁺	MoNA	1.49639E-05	Unknow	Phenols
45	M168T299	Phenylephrine	168.1017093	299.097	167.0946	C9H13NO2	C07441	[M+H] ⁺	BioDeepDB	4.96035E-08	Xenobiotics	Phenols
46	M136T449_2	Salicylamide	136.0410642	449.384	137.048	C7H7NO2	NULL	[M-H] ⁻	BioDeepDB	1.86242E-11	Unknow	Phenols
47	M121T437	Tyrosol	121.06564	437.161	138.0681	C8H10O2	C06044	[M+H-H2O] ⁺	BioDeepDB	4.54132E-08	Amino acid	Phenols