

Supplementary data

Table S1. Compound list

Compound	RT (min)	MSMS similarity	Area
<i>2,3,5,6-Tetramethylpyrazine</i>	6.286	97.8	23252576059.4
<i>Pipecolic acid</i>	1.557	88.2	16962426677.8
<i>Adenosine</i>	2.037	96.4	13092760204.6
<i>Betaine</i>	1.466	91.5	9765144346.1
<i>9-Oxo-10(E),12(E)-octadecadienoic acid</i>	22.112	91.5	8778321282.5
<i>Esculin</i>	7.136	88.3	7191291100.7
<i>Scopoletin</i>	7.405	89.6	6589184708.1
<i>Choline</i>	1.423	87.8	5816093510.1
<i>Hexadecanamide</i>	25.852	94	4802281361.2
<i>D,L-Camphor</i>	8.399	93.6	4539504142.0
<i>L-Phenylalanine</i>	3.565	96.1	4004785153.8
<i>L-Isoleucine</i>	2.328	85.7	3632272948.4
<i>Indole-3-acrylic acid</i>	6.476	93.3	3627603683.7
<i>7-Hydroxycoumarine</i>	7.002	94.7	3097087245.1
<i>Luteolin</i>	12.349	80.6	2877244051.6
<i>4-Guanidinobutyric acid</i>	1.897	91.9	2863865779.9
<i>Proline</i>	1.638	86.4	2252165470.6
<i>L-Norleucine</i>	2.194	84.5	2231210211.0
<i>Esculetin</i>	6.84	87.9	2014284782.1
<i>DL-Arginine</i>	1.399	90.9	1514149881.3
<i>2-Hydroxycinnamic acid</i>	2.096	88.2	1316662583.1
<i>Glycerophospho-N-palmitoyl ethanolamine</i>	21.336	75.3	1259469631.4
<i>Morin</i>	11.658	91.1	1152442324.5
<i>Apigenin</i>	13.412	95.4	1058778191.1
<i>Prolylleucine</i>	1.959	80.4	992470630.1
<i>Quercetin-3β-D-glucoside</i>	8.74	89.3	974293833.9
<i>Valine</i>	1.895	89.7	870666506.6
<i>Sedanolide</i>	14.078	74.4	852700142.4
<i>Nicotinamide</i>	1.907	92.4	812476208.6
<i>Eriodictyol</i>	8.336	75.1	765907026.5
<i>5α-Dihydrotestosterone</i>	22.918	81.8	749525529.9
<i>2-Amino-1,3,4-octadecanetriol</i>	19.756	73.4	749464263.5
<i>Daidzein</i>	23.061	85.3	749389562.3

<i>Nicotinic acid</i>	1.903	94.3	690434279.5
<i>Butein</i>	11.087	73	684289300.9
<i>Osajin</i>	19.175	74.7	655181530.9
<i>Isoliquiritigenin</i>	14.547	97.4	589212331.0
<i>Maltol</i>	5.271	92.4	509654616.6
<i>N-(2,4-Dimethylphenyl)formamide</i>	8.987	74.5	495202891.2
<i>Asparagine</i>	1.567	86.8	480269320.3
<i>N-α-L-Acetyl-arginine</i>	1.517	90.9	470380569.5
<i>Formononetin</i>	24.467	84.4	462091743.5
<i>Ethyl oleate</i>	23.867	85.5	456297249.0
<i>Mono(2-ethylhexyl) phthalate (MEHP)</i>	22.357	84.6	431506390.6
<i>Thymine</i>	2.272	85.5	409324195.0
<i>Adenine</i>	1.883	86.6	392298019.8
<i>19-Nortestosterone</i>	15.347	86.1	358119948.8
<i>Ursolic acid</i>	25.278	86.2	331350824.1
<i>Taxifolin</i>	8.704	87.8	318079047.9
<i>(\pm)-Abscisic acid</i>	6.665	82	312320913.6
<i>DL-Stachydrine</i>	2.125	85.1	308715206.7
<i>2'-O-Methyladenosine</i>	2.464	81.7	307468578.7
<i>2,6-Di-tert-butyl-1,4-benzoquinone</i>	16.263	70.2	282439446.1
<i>Alternariol</i>	10.334	74.8	272843113.9
<i>3-Succinoylpyridine</i>	6	71.7	259150576.9
<i>Resveratrol</i>	11.61	91.5	256913361.0
<i>α-Linolenoyl ethanolamide</i>	18.283	73	251212999.2
<i>Piceatannol</i>	18.624	81.8	239327352.3
<i>4-Acetamidobutanoic acid</i>	2.312	78.3	238796218.0
<i>Coumarin</i>	8.183	76.5	236230469.2
<i>Vanillin</i>	9.117	78	217152031.9
<i>8-Hydroxyquinoline</i>	10.657	89.5	198948175.7
<i>D-Glucosamine</i>	1.405	90.3	198922095.2
<i>Pyridoxine</i>	1.95475	86.9	194336849.5
<i>Citrinin</i>	13.703	71.5	194025789.1
<i>Uracil</i>	1.997	83.2	188221301.4
<i>Oleamide</i>	26.095	87.7	184056880.1
<i>Kojic acid</i>	5.543	86.4	180254958.3
<i>Palmitoleic acid</i>	25.888	86.7	174478300.6
<i>Estriol</i>	16.688	78.2	172035612.6
<i>Vitexin</i>	9.337	81.9	169889993.3

<i>trans-Cinnamaldehyde</i>	5.442	82.2	167977100.8
<i>Methyl cinnamate</i>	10.169	80.4	159884553.0
<i>Naringenin</i>	13.537	87	157819806.1
<i>Hypoxanthine</i>	2.118	83	149428042.3
<i>Purpurin</i>	11.052	79.4	149236385.0
<i>3-Methoxybenzaldehyde</i>	4.444	81.1	146455494.5
<i>Norfentanyl</i>	13.52	75.2	135939645.2
<i>Isophorone</i>	10.992	82.8	117000118.5
<i>Isorhamnetin</i>	12.016	84.2	115973391.9
<i>Trigonelline</i>	1.472	93.8	115942385.5
<i>8Z,11Z,14Z-Eicosatrienoic acid</i>	22.938	85.9	114726528.0
<i>Kuromanin</i>	10.409	82.1	112970307.4
<i>Nootkatone</i>	20.758	90.2	111785757.4
<i>3,4-Dihydroxybenzaldehyde</i>	9.58	85.9	107114123.4
<i>Emodin</i>	10.652	81.1	106612215.4
<i>Oxymatrine</i>	12.952	78.6	103455746.7
<i>2,3-Dihydroxybenzoic acid</i>	12.153	82.1	102202602.7
<i>Cuminaldehyde</i>	9.543	77.5	100338123.8
<i>Apocynin</i>	4.78	71.7	98155032.6
<i>Guanine</i>	1.883	88.4	96039704.0
<i>18-β-Glycyrrhetic acid</i>	20.982	92.3	95085329.7
<i>Polygodial</i>	21.439	81.3	93530786.5
<i>Kaempferol</i>	13.681	91.8	91488538.5
<i>6-Methylquinoline</i>	6.477	73.8	82755522.6
<i>Carvone</i>	15.02	89.2	72194810.1
<i>Biochanin A</i>	13.8	72.4	71148967.2
<i>2,6-Diethylaniline</i>	8.691	70.2	67662060.3
<i>2'-O-Methylguanosine</i>	2.775	81.4	67386521.1
<i>Chrysin</i>	18.155	84.9	67152653.8
<i>Glycitein</i>	16.565	90	65693330.1
<i>4-Hydroxybenzaldehyde</i>	8.335	79.6	64739878.4
<i>Chlorogenic acid</i>	5.914	90.1	59539551.7
<i>Icaritin</i>	19.544	80.6	57693801.2
<i>L-Histidine</i>	1.325	90	56662496.7
<i>Betulin</i>	19.202	85.4	55867864.3
<i>N-Acetyl-DL-tryptophan</i>	10.179	71.6	52911934.2
<i>Penicillic acid</i>	6	71.7	48774418.7
<i>4'-Methoxyacetophenone</i>	7.769	77.8	48540550.1
<i>4-Coumaric acid</i>	9.238	84.2	47549325.2

<i>Aflatoxin G1</i>	12.294	78.2	46496795.2
<i>Quercetin</i>	11.065	78.8	41805137.1
<i>Jasmonic acid</i>	13.328	76.3	41743852.2
<i>Arachidonic acid</i>	23.729	79.9	39228029.0
<i>Puerarin</i>	7.82	93	38199100.8
<i>Prunin</i>	10.569	86.1	34734343.0
<i>Acetophenone</i>	8.847	70.9	27001052.7
<i>Capsaicin</i>	12.386	71.6	26277452.5
<i>3-Acetyl-11-keto-β-boswellic acid</i>	21.537	72.6	13182932.9
<i>2-Hydroxybenzothiazole</i>	20.48	85.3	1977624.8
<i>Caprolactam</i>	19.875	86	1777756.9