

Supplementary Table 1 The criteria of DAI score.

Scores	Body weight loss	Diarrhea	Fecal blood
0	none	normal	no bleeding
1	1 %-5 %	—	—
2	6 %-10 %	loose stools	mild bleeding
3	11 %-20 %	—	—
4	over 20 %	watery diarrhea	severe bleeding

DAI = (Body weight loss score + Diarrhea score + Fecal blood score)/3.

Supplementary Table 2 The evaluation criterion of histological score.

Scores	Inflammation extent	Crypt aberrant	Lymphocyte infiltration	Colon wall aberrant
0	None	Normal	None	None
1	Slight	Basal 1/3 damaged	1%-25%	Mucosa
2	Moderate	Basal 2/3 damaged	26%-50%	Submucosa
3	Severe	Crypt lost and surface epithelium present	51%-75%	Transmural
4	—	Entire crypt and surface epithelium lost	76%-100%	—

Supplementary Table 3 UHPLC-Q-Orbitrap-HRMS of HZJDF

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
DL-Arginine	C6 H14 N4 O2	0.64	174.11179	175.11906	1.373	96.5	87.3	96.8	[M+H] ⁺ 1	7339725093
L-Aspartic acid	C4 H7 N O4	-0.14	133.03749	132.03021	1.376	86.3	37.4	93.1	[M-H] ⁻ 1	249929356.8
Asparagine	C4 H8 N2 O3	0.63	132.05358	133.06085	1.383	68.2	8.4	78.7	[M+H] ⁺ 1	301916398.7
α-D-Mannose 1-phosphate	C6 H13 O9 P	-0.51	260.02958	259.02231	1.389	76.5	52	82	[M-H] ⁻ 1	56089383.75
Kanosamine	C6 H13 N O5	0.12	179.07939	180.08667	1.4			70.3	[M+H] ⁺ 1	74949231.56
Choline	C5 H13 N O	0.41	103.09976	104.10703	1.423	95.9	9.8	91.8	[M+H] ⁺ 1	2462979668
Inositol	C6 H12 O6	-0.28	180.06334	179.05606	1.465	71.3	27.9	77.1	[M-H] ⁻ 1	281022901.7
L-(+)-Tartaric acid	C4 H6 O6	-0.85	150.01631	149.00903	1.485	91.6	45.1	92.3	[M-H] ⁻ 1	236535516.4
Quinic acid	C7 H12 O6	-0.08	192.06337	191.05609	1.494	89.1	78.9	89.5	[M-H] ⁻ 1	3239153796
D-Raffinose	C18 H32 O16	0.91	504.16949	549.16772	1.51	88.3	9.4	92.2	[M+FA-H] ⁻ 1	384192262.5
Sucrose	C12 H22 O11	0.04	342.11623	341.10889	1.515	95.4	58	94	[M-H] ⁻ 1	4119599227
Stachyose	C24 H42 O21	0.79	666.22238	665.21521	1.515			89.8	[M-H] ⁻ 1	161799659.7

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Proline	C5 H9 N O2	1.04	115.06345	116.07072	1.519	87.7	9.4	92	[M+H] ⁺ 1	3136699673
5-Hydroxymethyl-2-furaldehyde	C6 H6 O3	1.05	126.03183	127.03911	1.52	76.9	48.2	78.7	[M+H] ⁺ 1	398073595.8
Trigonelline	C7 H7 N O2	1.05	137.04782	138.0551	1.523	96.3	86.6	93.9	[M+H] ⁺ 1	437525613.1
DL-Stachydrine	C7 H13 N O2	1.12	143.09479	144.10207	1.528	90.6	9.5	74.3	[M+H] ⁺ 1	432166252.1
Maltopentaose	C30 H52 O26	0.25	828.27489	827.2677	1.533	67.7	26.9	90.9	[M-H] ⁻ 1	134310919.5
L-(-)-Malic acid	C4 H6 O5	-0.42	134.02147	133.01419	1.539	92.2	47.4	93.4	[M-H] ⁻ 1	4088592899
Fumaric acid	C4 H4 O4	-1.22	116.01082	115.00354	1.54	84.2	9.2	96.1	[M-H] ⁻ 1	574571230.7
Phenibut	C10 H13 N O2	0.98	179.0948	180.10208	1.54	72.8	52	61.1	[M+H] ⁺ 1	209691572.1
Adenine	C5 H5 N5	0.99	135.05463	136.0619	1.542	79.9	9	82.9	[M+H] ⁺ 1	218423980.7
trans-Aconitic acid	C6 H6 O6	-0.79	174.0163	173.009	1.582	82.1	70.7	88.6	[M-H] ⁻ 1	398235966.7
2-Furoic acid	C5 H4 O3	-1.1	112.01592	111.00864	1.642	93.2	50.8	90.3	[M-H] ⁻ 1	952496774.9
Itaconic acid	C5 H6 O4	-0.11	130.02659	129.01932	1.642	90.6	9.5	100	[M-H] ⁻ 1	159727511.7

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Citric acid	C6 H8 O7	0.18	192.02704	191.01976	1.647	86.6	58.5	96	[M-H]-1	11341123431
D-(+)-Pyroglutamic Acid	C5 H7 N O3	0.92	129.04271	130.04999	1.841	84.3	9.2	88.3	[M+H]+1	1275957418
α,α -Trehalose	C12 H22 O11	0.04	342.11623	341.10889	1.941	95.5	58.3	95.1	[M-H]-1	2171235286
Maleic acid	C4 H4 O4	-1.22	116.01082	115.00354	2.049	61.7	8.1	87.9	[M-H]-1	289257898.8
Shikimic acid	C7 H10 O5	-0.69	174.0527	173.04543	2.253	91.3	82	88.7	[M-H]-1	237545019
Uridine monophosphate (UMP)	C9 H13 N2 O9 P	0.3	324.03596	323.02869	2.395	78.1	8.9	81.8	[M-H]-1	57170407.36
Pipecolic acid	C6 H11 N O2	1.56	129.07918	130.08646	2.405	77.2	8.9	75.8	[M+H]+1	259229610.3
Nicotinic acid	C6 H5 N O2	1.32	123.03219	124.03947	2.622	89.3	9.5	92.5	[M+H]+1	314895555.5
4-Guanidinobutyric acid	C5 H11 N3 O2	0.87	145.08525	146.09253	2.667	91.1	82.8	88	[M+H]+1	182408496
Cytosine	C4 H5 N3 O	0.95	111.04337	112.05064	2.776	68.2	43.9	79.2	[M+H]+1	92750165.43
Adenine	C5 H5 N5	0.99	135.05463	136.0619	2.786	93.9	9.7	95.6	[M+H]+1	691489929.9
Guanine	C5 H5 N5 O	0.61	151.0495	152.05678	2.817	90.9	9.5	88.2	[M+H]+1	167479982

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Acetylarginine	C8 H16 N4 O3	0.78	216.12241	217.12968	2.828	86.7	80	74.6	[M+H] ⁺ 1	78211193.35
Argininosuccinic acid	C10 H18 N4 O6	0.32	290.12273	291.13	2.941	78.3	73.9	58.9	[M+H] ⁺ 1	240643874.8
Phenylalanine	C9 H11 N O2	1.13	165.07916	166.08644	3.036	60.7	42.7	74.5	[M+H] ⁺ 1	156624839.2
Adenosine 5'-monophosphate	C10 H14 N5 O7 P	0.48	347.06325	348.07053	3.158	76.6	8.8	82.8	[M+H] ⁺ 1	116269312.1
Nicotinamide	C6 H6 N2 O	0.57	122.04808	123.05536	3.174	90.5	9.5	89	[M+H] ⁺ 1	221197271.7
4-Aminophenol	C6 H7 N O	1.08	109.05288	110.06016	3.322	62	8.1	86.8	[M+H] ⁺ 1	72853924.1
Pyrrole-2-carboxylic acid	C5 H5 N O2	0.22	111.03205	112.03933	3.325			71.9	[M+H] ⁺ 1	62621302.83
L-Pyroglutamic acid	C5 H7 N O3	0.63	129.04267	130.04999	3.439	91.7	9.6	97.7	[M+H] ⁺ 1	1731729837
Guanosine monophosphate (GMP)	C10 H14 N5 O8 P	1.17	363.05842	362.05115	3.601	78.8	32.6	88.7	[M-H] ⁻ 1	21649578.1
Uric acid	C5 H4 N4 O3	0.23	168.02838	167.02106	3.627	92.2	9.6	91.1	[M-H] ⁻ 1	27991052.49
L-Norleucine	C6 H13 N O2	0.88	131.09474	132.10202	4.149	80.8	9	84.9	[M+H] ⁺ 1	705569319.1

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
3-Butene-1,2,3- tricarboxylic acid	C7 H8 O6	0.57	188.03219	187.02492	4.28	69.8	47.7	73.8	[M-H]-1	30758102.63
Salsolinol	C10 H13 N O2	0.98	179.0948	180.10208	4.334	77.9	58.9	63.4	[M+H]+1	526885815.1
L-Tyrosine	C9 H11 N O3	0.97	181.07407	182.08134	4.947	88.8	81.6	89.8	[M+H]+1	159685672.5
Uridine	C9 H12 N2 O6	0.1	244.06956	243.06224	5.067	85.7	57.9	96.3	[M-H]-1	197699176.2
Thymidine 5'-monophosph ate	C10 H15 N2 O8 P	0.45	322.05675	321.04947	6.136	78.2	66.1	88.8	[M-H]-1	12584744.06
Gallic acid	C7 H6 O5	0.21	170.02156	169.01427	7.446	97.9	9.9	97.7	[M-H]-1	5393398801
Pyrogallol	C6 H6 O3	-0.81	126.03159	125.02431	7.481	83.3	9.2	90.4	[M-H]-1	1192842121
Guanosine-3',5' -cyclic monophosphate	C10 H12 N5 O7 P	0.28	345.04753	344.04025	7.794			78.2	[M-H]-1	85115314.58
Adenosine	C10 H13 N5 O4	0.5	267.09689	268.10416	10.034	90.8	9.5	92	[M+H]+1	1111453921
L-Phenylalanin e	C9 H11 N O2	1.13	165.07916	166.08644	11.183	87.2	9.4	92.4	[M+H]+1	808090797.3

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Maltol	C6 H6 O3	0.88	126.03181	127.03911	15.405	86	53.6	91.3	[M+H] ⁺ 1	101862647.3
TDIQ	C10 H11 N O2	1.22	177.07919	178.08647	15.763	82.3	64.9	65.8	[M+H] ⁺ 1	45615526.02
2,3-Dihydroxybenzoic acid	C7 H6 O4	0.01	154.02661	153.01933	15.835	94	9.7	96.9	[M-H] ⁻ 1	190215816.4
Catechol	C6 H6 O2	-1.11	110.03666	109.02938	15.844	89.1	9.5	76.4	[M-H] ⁻ 1	44406258.38
Danshensu	C9 H10 O5	0.31	198.05288	197.04561	15.967			88.5	[M-H] ⁻ 1	150618592.3
Pantothenic acid	C9 H17 N O5	0.79	219.11084	220.11819	16.402	68.9	44	81.2	[M+H] ⁺ 1	49965907.49
Kojic acid	C6 H6 O4	1	142.02675	143.03403	16.421	80.4	50.3	80	[M+H] ⁺ 1	32461035.13
Penicillic acid	C8 H10 O4	0.45	170.05799	171.06526	16.73	75.3	71.8	68.1	[M+H] ⁺ 1	30625715.77
2,5-DMMA	C12 H19 N O2	0.34	209.14165	210.14893	16.768			77.1	[M+H] ⁺ 1	139964372.7
4-Hydroxybenzoic acid	C7 H6 O3	0	138.03169	139.03897	16.838	79.5	61.1	67.7	[M+H] ⁺ 1	47851264.92
Epigallocatechin (-)	C15 H14 O7	0.52	306.07411	305.06683	16.841			94.5	[M-H] ⁻ 1	468209783.7
1-Caffeoylquinic acid	C16 H18 O9	0.15	354.09514	353.08786	16.858	83.8	35.8	85.1	[M-H] ⁻ 1	15841720.92

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Isovanillic acid	C8 H8 O4	-0.14	168.04223	167.03496	16.904	90.4	40.9	91.3	[M-H]-1	40804410.23
3,4-Dihydroxyphenylethanol	C8 H10 O3	-0.05	154.06299	153.05571	16.984	75.5	8.8	81.5	[M-H]-1	41546985.72
o-Veratraldehyde	C9 H10 O3	1.26	166.0632	167.07048	17.05	77.9	8.9	65.2	[M+H]+1	64967474.47
3-Hydroxybenzyl alcohol	C7 H8 O2	0.04	124.05244	123.04516	17.057	76.6	8.8	82.5	[M-H]-1	28680044.6
Caftaric acid	C13 H12 O9	0.61	312.04832	311.04105	17.38	82.8	35.2	91.2	[M-H]-1	354128492.7
Caffeic acid	C9 H8 O4	-0.13	180.04223	179.03496	17.394	92.3	9.6	93.4	[M-H]-1	140203233
Geraniin	C41 H28 O27	0.62	952.08239	951.07513	17.437			74.1	[M-H]-1	87841130.55
6-Methylquinoline	C10 H9 N	0.14	143.07352	144.0808	17.461	84.7	9.2	69.2	[M+H]+1	145118076.7
1,5-Naphthalenediamine	C10 H10 N2	0.58	158.08449	159.09177	17.462	82.8	65.7	84.2	[M+H]+1	26796564.7
trans-3-Indoleacrylic acid	C11 H9 N O2	0.39	187.0634	188.07068	17.467	96.2	86.4	92.9	[M+H]+1	728224986.9
L-Tryptophan	C11 H12 N2 O2	0.6	204.09	205.09727	17.469	94.4	71.6	92.3	[M+H]+1	455396750.9
Bioside	C20 H30 O12	1.31	462.17433	461.16705	17.518	80.5	9	79.3	[M-H]-1	111994418.7

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Quinic acid	C7 H12 O6	-0.1	192.06337	191.05609	17.52	83.4	56.4	83.8	[M-H]-1	49513091.04
Chlorogenic acid	C16 H18 O9	0.19	354.09515	353.08786	17.53	90.7	42.1	91.2	[M-H]-1	1709371509
Methylgallate	C8 H8 O5	0.22	184.03721	183.02994	17.562			74.1	[M-H]-1	47640633.35
Leucylproline	C11 H20 N2 O3	0.38	228.14748	229.15475	17.576	82.1	51.3	81.2	[M+H]+1	43360999.31
5'-S-Methyl-5'-t hioadenosine	C11 H15 N5 O3 S	0.5	297.08971	298.09698	17.662	82.3	51.4	83.9	[M+H]+1	80754882.68
Shanzhiside methyl ester	C17 H26 O11	-0.39	406.14735	405.14008	17.68	68	26.9	72.8	[M-H]-1	39264504.9
3,5-Dimethyl-4- methoxybenzoic acid	C10 H12 O3	0.6	180.07875	181.08603	17.683	78.6	74.2	69.3	[M+H]+1	44000056.17
2,5-Dihydroxybenzaldehyde	C7 H6 O3	-0.36	138.03164	137.02437	17.773	94	9.7	90.5	[M-H]-1	390505121.5
Phenylacetaldehyde	C8 H8 O	-0.88	120.05741	119.05013	17.843	75.6	8.8	66.9	[M-H]-1	37892287.61
Xanthurenic acid	C10 H7 N O4	0.67	205.03765	206.04492	17.845	82.3	51.4	80.9	[M+H]+1	34457652.15
Loganic acid	C16 H24 O10	0.57	376.13716	375.12988	17.924	88.1	77.7	88.2	[M-H]-1	273247380.9

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Ellagic acid	C14 H6 O8	0.12	302.0063	303.01358	17.932	74.7	46.9	76.5	[M+H] ⁺ 1	58749186.91
Corilagin	C27 H22 O18	0.91	634.08119	633.07391	17.948			86.2	[M-H] ⁻ 1	486408482.5
Kynurenic acid	C10 H7 N O3	0.38	189.04267	190.04994	17.986	85.3	9.3	51.5	[M+H] ⁺ 1	68938846.59
4-Phenylbutyric acid	C10 H12 O2	0.36	164.08379	165.09106	17.995	84.4	78.4	86.6	[M+H] ⁺ 1	71822890.38
Indole-3-carbox aldehyde	C9 H7 N O	0.34	145.05281	146.06009	18.004	75	8.8	82.3	[M+H] ⁺ 1	20464838.15
2-Isopropylmali c acid	C7 H12 O5	-0.66	176.06836	175.06108	18.1	92.7	9.6	92.9	[M-H] ⁻ 1	85569749.78
Esculin	C15 H16 O9	0.03	340.07944	339.07211	18.105	90.9	9.5	94.3	[M-H] ⁻ 1	9510798856
Esculetin	C9 H6 O4	0.07	178.02662	179.03398	18.105	95.9	85.6	94.7	[M+H] ⁺ 1	1332412625
1-Naphthol	C10 H8 O	0.41	144.05757	145.06485	18.177			85.4	[M+H] ⁺ 1	16352605.53
Methyl cinnamate	C10 H10 O2	0.04	162.06809	163.07536	18.284	73.4	46.2	78.6	[M+H] ⁺ 1	58651734.19
Methyl gallate	C8 H8 O5	-0.11	184.03715	183.02988	18.303			91.9	[M-H] ⁻ 1	223242226.9
Fraxetin	C10 H8 O5	-0.08	208.03716	209.04443	18.333	67.6	67.2	71.3	[M+H] ⁺ 1	38325905.23

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1,6-Bis-O-(3,4, 5-trihydroxyben zoyl)hexopyran ose	C20 H20 O14	0.68	484.08563	483.07837	18.349	91.4	82.1	89.8	[M-H]-1	729198038.3
Gentiopictin	C16 H20 O9	0.59	356.11094	355.10364	18.468			73.3	[M-H]-1	49425667.75
Isoferulic acid	C10 H10 O4	-0.25	194.05786	193.05055	18.471	83	56.2	90.1	[M-H]-1	23664608.12
Forsythoside E	C20 H30 O12	0.95	462.17417	461.1669	18.546	76.9	8.8	75.8	[M-H]-1	98581725.78
Procyanidin B1	C30 H26 O12	0.64	578.1428	577.13556	18.558			91.4	[M-H]-1	1726175415
Oxypaeoniflori n	C23 H28 O12	0.53	496.15834	495.15106	18.661	74.8	30.1	93	[M-H]-1	180835852
BMK methyl glycidate	C11 H12 O3	0.25	192.07869	193.08597	18.674	78.3	8.9	80.3	[M+H]+1	392316896.7
Terephthalic acid	C8 H6 O4	-0.73	166.02649	165.01921	18.795	84.1	9.2	88	[M-H]-1	209729991.5
Coumarin	C9 H6 O2	-0.13	146.03676	147.04404	18.796	77.6	8.9	77.3	[M+H]+1	251127099.4
Benzoic acid	C7 H6 O2	-0.41	122.03673	123.04401	18.8	86.6	9.3	87.1	[M+H]+1	712574124.6
Naringenin chalcone	C15 H12 O5	-0.58	272.06832	273.07559	18.8	78.3	74	74.8	[M+H]+1	407281079

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3,4-Dihydroxybenzaldehyde	C7 H6 O3	-0.03	138.03169	139.03897	18.801	84.5	68	79.9	[M+H] ⁺ 1	2386731477
4-Coumaric acid	C9 H8 O3	0.22	164.04738	165.05466	18.807	92.2	63.9	91	[M+H] ⁺ 1	249416039.7
2-Naphthylamine	C10 H9 N	0.14	143.07352	144.0808	18.815	86.4	9.3	73.8	[M+H] ⁺ 1	299069567.8
Catechin	C15 H14 O6	0	290.07904	289.07181	18.816	94.7	87.3	95.7	[M-H] ⁻ 1	35766128475
2,3,4,9-Tetrahydro-1H-β-carboline-3-carboxylic acid	C12 H12 N2 O2	0.06	216.08989	217.09717	18.816	85.5	53.3	89.4	[M+H] ⁺ 1	219840693.7
(-)-Gallocatechin	C15 H14 O7	0.51	306.07411	305.06683	18.857			84.6	[M-H] ⁻ 1	120407815.2
Cryptochlorogenic acid	C16 H18 O9	0.19	354.09515	353.08786	18.918	91.9	46.4	93.1	[M-H] ⁻ 1	2828502169
4-Hydroxymandelic acid	C8 H8 O4	-0.33	168.0422	167.03493	19.008	88	9.4	89.8	[M-H] ⁻ 1	283379163.8
4-Hydroxybenzylalcohol	C7 H8 O2	-0.45	124.05237	123.0451	19.008	74.7	8.7	52.6	[M-H] ⁻ 1	79814440.09
Procyanidin B2	C30 H26 O12	0.56	578.14275	579.15002	19.009			89.3	[M+H] ⁺ 1	451800711.2

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Ethyl 4-(2-methoxyph enyl)piperazine -1-carboxylate	C14 H20 N2 O3	-0.25	264.14733	265.1546	19.03	75.5	47.5	51.2	[M+H]+1	28701398.93
Fraxin	C16 H18 O10	0.2	370.09007	369.08279	19.262	87	9.4	89.1	[M-H]-1	4734715343
Fraxetin	C10 H8 O5	-0.08	208.03716	209.04443	19.268	90.2	82.5	91	[M+H]+1	6771792632
Phellodendrine chloride			341.16265	342.16992	19.401			71.3	[M+H]+1	15839218.46
6,7-Dihydroxyc oumarin	C9 H6 O4	0.04	178.02662	177.01932	19.402			90.3	[M-H]-1	2428496238
3',4'-Dihydroxy phenylacetone	C9 H10 O3	1.26	166.0632	167.07048	19.441	79.9	9	76	[M+H]+1	24474348.75
2-Methylbenzoi c acid	C8 H8 O2	-0.13	136.05241	135.04514	19.497	81.9	9.1	61.6	[M-H]-1	151929667.3
Brevifolincarbo xylic acid	C13 H8 O8	-0.38	292.02181	293.02908	19.529			78.6	[M+H]+1	52292004.41
Vicenin II	C27 H30 O15	0.81	594.15895	595.16614	19.604	73.8	46.4	83	[M+H]+1	31891524.74
Cantharidin	C10 H12 O4	-0.02	196.07355	197.08083	19.698	80.2	75.3	72	[M+H]+1	173919263

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
5-Hydroxymethylfurfural	C6 H6 O3	1.09	126.03183	127.03911	19.698	73.4	8.7	81.9	[M+H] ⁺ 1	40560686
Riboflavin	C17 H20 N4 O6	-0.22	376.1382	377.14548	19.705	84.4	9.2	88.7	[M+H] ⁺ 1	60798997.27
Naringenin	C15 H12 O5	-0.58	272.06832	273.07559	19.79	76	56.2	76.2	[M+H] ⁺ 1	97674117.76
Ferulic acid	C10 H10 O4	-0.43	194.05782	193.05054	19.838	93.1	50.4	94	[M-H] ⁻ 1	278687707.7
Methyl 4-hydroxy-3-methoxycinnamate	C11 H12 O4	0.39	208.07364	209.08092	19.869	74.9	71.5	69.1	[M+H] ⁺ 1	49536627.28
Pinoresinol diglucoside	C32 H42 O16	1.24	682.24813	727.2464	19.921	73.9	8.7	88.8	[M+FA-H] ⁻ 1	154306323.2
Noreugenin	C10 H8 O4	0.58	192.04237	193.04964	19.922	79.3	9	56.2	[M+H] ⁺ 1	30835517.73
1,3-Dicaffeoylquinic acid	C25 H24 O12	-1.49	516.12601	515.11865	20.048	88.5	38.8	91.4	[M-H] ⁻ 1	403310076.8
Acetophenone	C8 H8 O	-0.09	120.0575	121.06478	20.067	82.5	51.5	84.5	[M+H] ⁺ 1	51461393.88
Plantamajoside	C29 H36 O16	0.85	640.20088	639.1936	20.107			84.8	[M-H] ⁻ 1	47248205.08
Taxifolin	C15 H12 O7	-0.29	304.05821	305.06549	20.122	91.3	82.9	90.6	[M+H] ⁺ 1	38231100.76

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
(+)-Magnoflorine	C20 H23 N O4	-0.15	341.16266	342.16992	20.136	81.4	50.9	89	[M+H] ⁺ 1	7604177689
Secoxyloganin	C17 H24 O11	0.57	404.13209	403.12482	20.197	76.3	31.1	93.6	[M-H] ⁻ 1	87833453.42
Syringic acid	C9 H10 O5	-0.21	198.05278	197.0455	20.277	78.9	53.5	80.9	[M-H] ⁻ 1	1304409040
Vicenin III	C26 H28 O14	0.49	564.14818	565.15546	20.29	63.6	66	80.1	[M+H] ⁺ 1	148723265.6
Fraxinellone	C14 H16 O3	-0.08	232.10993	233.1172	20.33	74.8	71.4	78.7	[M+H] ⁺ 1	57193881.01
Paeoniflorin	C23 H28 O11	0.52	480.16341	525.16162	20.45	79.7	9	95.5	[M+FA-H] ⁻ 1	10338304493
2,4-Dimethylbenzaldehyde	C9 H10 O	-0.09	134.07315	135.08043	20.47	68.3	67.4	81.8	[M+H] ⁺ 1	135547211.8
4-Methoxycinnamic acid	C10 H10 O3	-0.02	178.06299	179.07027	20.471	65.5	66.6	72.3	[M+H] ⁺ 1	1292315357
3,4-Dimethylbenzoic acid	C9 H10 O2	0.25	150.06812	151.07539	20.471	78.5	74.1	75.3	[M+H] ⁺ 1	1019655717
7-Methoxycoumarin	C10 H8 O3	0.38	176.04741	177.05469	20.568	83	77.3	78.1	[M+H] ⁺ 1	571215201.1
D-(-)-Quinic acid	C7 H12 O6	0.13	192.06341	191.05614	20.581	87.8	9.4	84.5	[M-H] ⁻ 1	117531402.6
Benzidine	C12 H12 N2	0.44	184.10013	185.10741	20.588	77.4	48.5	75.5	[M+H] ⁺ 1	151461786.4

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Luteolin-3',7-Di glucoside	C27 H30 O16	0.82	610.15388	609.14673	20.723	83.2	51.9	82.4	[M-H]-1	49803457.32
Grosvenorine	C33 H40 O19	1.07	740.21717	739.21008	20.797	87.4	9.4	87.1	[M-H]-1	510505922.4
Kaempferol-3- O-rutinoside	C27 H30 O15	0.66	594.15886	595.16614	20.811	85.5	53.3	84.9	[M+H]+1	97027891.08
N-Acetyl-L-phe nylalanine	C11 H13 N O3	0.12	207.08957	206.08229	20.861	85.3	36.7	89.2	[M-H]-1	53587120.8
Vanillin	C8 H8 O3	0.64	152.04744	153.05472	20.902	70.8	68.5	80.3	[M+H]+1	29004366.58
Linderalactone	C15 H16 O3	0.24	244.11	245.11728	20.967			73.2	[M+H]+1	25144284.96
3-Phenyllactic acid	C9 H10 O3	-0.23	166.06296	165.05568	21.034	83.8	56.6	90.4	[M-H]-1	26085627.02
Isoquercitrin	C21 H20 O12	0.66	464.09578	465.10306	21.046	85.6	9.3	82.8	[M+H]+1	70015565.53
4-Vinylphenol	C8 H8 O	-0.62	120.05744	119.05016	21.144	89.9	9.5	77.3	[M-H]-1	72144424.43
Lusitanicoside	C21 H30 O10	0.93	442.18431	441.17703	21.155	76.5	64.1	65.9	[M-H]-1	23022673.56
Rutin	C27 H30 O16	0.88	610.15392	609.14673	21.239	85.9	37.1	92.3	[M-H]-1	523879407.4
Leucoside	C26 H28 O15	0.03	580.14284	581.15057	21.264	76.7	48.2	65.1	[M+H]+1	52363915.42

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Lariciresinol 4-O-glucoside	C26 H34 O11	1.01	522.21064	567.20886	21.315	87.3	38	84.6	[M+FA-H]- 1	181774066.6
Papaverine	C20 H21 N O4	0.16	339.14711	340.15439	21.32	71.1	49.5	66.2	[M+H]+1	236238181.6
Lonicerin	C27 H30 O15	0.66	594.15886	595.16614	21.356	80.1	50.1	85.6	[M+H]+1	139753113
Eriodictyol	C15 H12 O6	-0.27	288.06331	289.07059	21.358	80.5	62.5	77.4	[M+H]+1	51509925.31
Vitexin	C21 H20 O10	0.51	432.10587	433.11319	21.368			76	[M+H]+1	24172756.79
Verbascoside	C29 H36 O15	1.04	624.20607	623.19879	21.422	89.9	39.7	91.2	[M-H]-1	94703808.06
(-)-Epicatechin gallate	C22 H18 O10	0.58	442.09025	441.08298	21.426			84.2	[M-H]-1	64810204.66
Glaucine	C21 H25 N O4	0.01	355.17836	356.18564	21.514	71.2	8.6	54	[M+H]+1	273438935.4
Cichoric acid	C22 H18 O12	0.56	474.08009	473.07281	21.516			92.7	[M-H]-1	648676953.7
Quercetin-3β-D -glucoside	C21 H20 O12	0.74	464.09582	463.08856	21.613	89.8	60.5	96	[M-H]-1	1829389969
Quercetin	C15 H10 O7	-0.01	302.04265	303.04993	21.613	97.3	95.1	92.9	[M+H]+1	1057934278
Calceolarioside B	C23 H26 O11	0.19	478.1476	477.14032	21.701			92.6	[M-H]-1	1733001652

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Skimmin	C15 H16 O8	-0.37	324.0844	325.09167	21.702			72.6	[M+H] ⁺ 1	163844092.5
Cynaroside	C21 H20 O11	0.49	448.10078	449.10794	21.732	84.4	52.6	80.1	[M+H] ⁺ 1	123115517.1
Poncirin	C28 H34 O14	-2.19	594.19356	593.18628	21.753			72.3	[M-H] ⁻ 1	23063402.69
Kaempferol 3-glucorhamnoside	C27 H30 O15	0.88	594.15899	593.15179	21.763	84.4	9.2	86.4	[M-H] ⁻ 1	163803641.3
Ellagic acid	C14 H6 O8	-0.19	302.00621	300.99893	21.766			89.4	[M-H] ⁻ 1	1489267343
Scopoletin	C10 H8 O4	0.53	192.04236	193.04964	21.766	93.3	9.7	91.5	[M+H] ⁺ 1	211199312.3
Naringin dihydrochalcone	C27 H34 O14	1.44	582.19569	581.18842	21.785			75.4	[M-H] ⁻ 1	19323344.14
(-)-Catechin gallate	C22 H18 O10	0.58	442.09025	441.08298	21.819			88.1	[M-H] ⁻ 1	190344782
Yohimbine	C21 H26 N2 O3	-0.14	354.19429	355.20157	21.898	83.9	52.3	82.9	[M+H] ⁺ 1	171856948.9
Isoacteoside	C29 H36 O15	1.03	624.20606	623.19879	21.96	89.4	39.3	90.9	[M-H] ⁻ 1	294172743.8
Isofraxidin	C11 H10 O5	-0.18	222.05278	223.06004	22.04	77.8	73.6	83	[M+H] ⁺ 1	66482510.93

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
4,5-Dicaffeoylquinic acid	C25 H24 O12	0.73	516.12715	515.11987	22.07	90.9	42.9	90.7	[M-H]-1	615021955.3
(+)-Pinoresinol	C20 H22 O6	0.11	358.14168	357.1344	22.082			85.5	[M-H]-1	56494922.4
Pinoresinol										
4-O-glucoside	C26 H32 O11	0.66	520.19481	519.1875	22.084	87.5	38.2	87.7	[M-H]-1	325874653.4
(+)										
Citral	C10 H16 O	0.33	152.12016	153.12744	22.126			70.2	[M+H]+1	27940573.28
5-O-Methylvisammioside	C22 H28 O10	0.23	452.16835	453.17563	22.158	78.4	59.7	79.6	[M+H]+1	22230877.37
Kaempferol	C15 H10 O6	-0.08	286.04772	287.05499	22.196	91.2	77.4	86.3	[M+H]+1	267546744.4
Astragalin	C21 H20 O11	0.62	448.10084	447.09366	22.199	86	58.1	91.1	[M-H]-1	313028360.8
Demethyleneberberine	C19 H17 N O4	-1.17	323.11538	324.12265	22.27			88	[M+H]+1	1040556264
Berberrubine	C19 H15 N O4	-0.07	321.10008	322.10736	22.287			83.6	[M+H]+1	3802972589
Naringin	C27 H32 O14	1.38	580.18001	579.17273	22.307	70.8	48.3	65.3	[M-H]-1	26538675.11
Rhoifolin	C27 H30 O14	0.49	578.16384	579.17084	22.395	78.1	8.9	81.2	[M+H]+1	27713979.74
3,5-Dicaffeoylquinic acid	C25 H24 O12	0.72	516.12715	515.11987	22.434	90.2	40.5	91.7	[M-H]-1	327478674.7

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Kaempferol	C15 H10 O6	-0.08	286.04772	287.05499	22.451	94.9	9.7	89.3	[M+H] ⁺ 1	302105179.4
Astragalin	C21 H20 O11	0.61	448.10083	447.09366	22.459	77.7	52.7	84.1	[M-H] ⁻ 1	457189023
10-Hydroxyliqu stroside	C25 H32 O13	0.77	540.18471	539.17743	22.464	92.1	67.6	87.3	[M-H] ⁻ 1	52736198.06
Oxoglaucine	C20 H17 N O5	0	351.11067	352.11795	22.549			78.9	[M+H] ⁺ 1	620129847.3
Isorhamnetin-3- glucoside	C22 H22 O12	0.61	478.11142	477.10419	22.556			85	[M-H] ⁻ 1	123903493.3
Dehydroglauцин e	C21 H23 N O4	-0.18	353.16265	354.16992	22.601			78.4	[M+H] ⁺ 1	372197866.3
Apigetrin	C21 H20 O10	0.84	432.10601	433.11319	22.683	78.8	8.9	82.6	[M+H] ⁺ 1	33588737.28
Indole	C8 H7 N	0.31	117.05789	118.06516	22.881			74.9	[M+H] ⁺ 1	63502348.35
Albiflorin	C23 H28 O11	0.4	480.16335	525.16162	22.882	90.4	57.4	90.3	[M+FA-H] ⁻ 1	3596281760
trans-Cinnamal dehyde	C9 H8 O	-0.02	132.05751	133.06479	22.883	85.1	78.9	86.8	[M+H] ⁺ 1	444916987
Xanthoxylene	C10 H12 O4	-0.05	196.07355	197.08083	22.884	84.1	78.2	78.1	[M+H] ⁺ 1	1319585176
Azelaic acid	C9 H16 O4	0.32	188.10492	187.09764	22.986	91.1	9.6	93.1	[M-H] ⁻ 1	138411611.8

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Rosmarinic acid	C18 H16 O8	0.68	360.08476	359.07748	23.03	63	8.1	84.6	[M-H]-1	233133539.4
1,2,3,4,6-Penta galloylglucose	C41 H32 O26	0.42	940.11858	469.05194	23.101			91.7	[M-2H]-2	465558943.9
1,2,3,4,6-O										
Phloridzin	C21 H24 O10	0.56	436.13719	435.12991	23.123			88.9	[M-H]-1	66442936.02
Dihydropalmati ne	C21 H23 N O4	-0.18	353.16265	354.16992	23.176			71.7	[M+H]+1	38394706.58
Salicylic acid	C7 H6 O3	-0.36	138.03164	137.02437	23.203	89.3	9.5	93.8	[M-H]-1	114535678.9
4-Methoxybenz aldehyde	C8 H8 O2	0.14	136.05245	137.05972	23.23	65.9	47.3	77.5	[M+H]+1	265453487.7
Oleuropein	C25 H32 O13	0.87	540.18476	539.17749	23.262	65	26.6	92.5	[M-H]-1	1090279821
Jatrorrhizine	C20 H19 N O4	-0.85	337.13112	338.1384	23.328			91.2	[M+H]+1	14599815786
Coptisine chloride			319.0844	320.09167	23.637			89.1	[M+H]+1	16938027613
Baicalin	C21 H18 O11	0.11	446.08496	447.0921	23.731	84	9.2	87.9	[M+H]+1	458999234.5
5,7,8-Trihydrox yflavone	C15 H10 O5	-1.47	270.05243	271.05966	23.732	84.3	52.6	86.5	[M+H]+1	49213814.19

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Nabumetone	C15 H16 O2	0.04	228.11504	229.12231	23.897	87.9	80.9		[M+H] ⁺ 1	43525732.94
Scoparone	C11 H10 O4	0.08	206.05792	207.0652	23.948	80.5	75.5	80.4	[M+H] ⁺ 1	19315655.75
Parthenolide	C15 H20 O3	0.28	248.14131	249.14859	24.395	85	78.8	85.2	[M+H] ⁺ 1	39917532.71
Phenylacetalde hyde	C8 H8 O	-0.1	120.0575	121.06478	24.486	82.6	51.6	88.5	[M+H] ⁺ 1	74100140.15
Baicalin	C21 H18 O11	0.26	446.08503	447.0921	24.56	81.5	9.1	85.1	[M+H] ⁺ 1	35614556.07
Palmatine	C21 H21 N O4	-0.8	351.14678	352.15405	24.738			92.1	[M+H] ⁺ 1	25297317816
Liquiritigenin	C15 H12 O4	0.25	256.07362	255.06635	24.921			83.2	[M-H] ⁻ 1	8307040.831
Berberine	C20 H17 N O4	-0.51	335.11559	336.12286	24.942	96.3	9.8	95.9	[M+H] ⁺ 1	85826586265
Oroxylin A-7-O-β-D-glu curonide	C22 H20 O11	0.61	460.10084	459.09357	25.028			92.8	[M-H] ⁻ 1	39389274.74
Buddlejasaponi n IVb	C48 H78 O18	-0.74	942.51811	943.52539	25.279	87.6	54.5	78.5	[M+H] ⁺ 1	84339740.48
Luteolin	C15 H10 O6	-0.02	286.04773	287.05493	25.447	85.6	9.3	82.3	[M+H] ⁺ 1	72023559.06
Dehydrocorydal ine	C22 H23 N O4	0.16	365.16277	366.17004	25.533	68.5	8.4	86.9	[M+H] ⁺ 1	258913952.2

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Wogonoside	C22 H20 O11	0.6	460.10084	461.10803	25.599	83.8	9.2	82.3	[M+H] ⁺ 1	177721814.6
Benzoylpaeonif lorin	C30 H32 O12	0.5	584.18967	629.18787	26.34			94.1	[M+FA-H] ⁻ 1	990698649.8
Ferulaldehyde	C10 H10 O3	-0.02	178.06299	179.07027	26.342	75.5	71.9	69.1	[M+H] ⁺ 1	29654120.53
Mesterolone	C20 H32 O2	0.87	304.2405	305.24777	26.814	73.8	70.7	71.8	[M+H] ⁺ 1	9516158.92
Pedunculoside	C36 H58 O10	1.01	650.40365	695.40186	26.934	76.1	30.9	76.4	[M+FA-H] ⁻ 1	83717258.32
Phloretin	C15 H14 O5	0.42	274.08424	273.07697	26.957	83	9.2	91.7	[M-H] ⁻ 1	30228651.22
9S,13R-12-Oxo phytodienoic acid	C18 H28 O3	0	292.20384	293.21112	26.995	85.7	79.3	81.8	[M+H] ⁺ 1	42101972.31
Corchorifatty acid F	C18 H32 O5	0.42	328.22511	327.21783	26.999	89.9	79.8	87.2	[M-H] ⁻ 1	271581273.1
19-Nortestoster one	C18 H26 O2	0.46	274.19341	275.20068	27	90.2	82.5	75.2	[M+H] ⁺ 1	62270840.02
Matairesinol	C20 H22 O6	0.68	358.14188	357.13467	27.122	86.5	75.9	86.2	[M-H] ⁻ 1	37418922.83
Genistein	C15 H10 O5	0.4	270.05293	269.04565	27.26	82.8	9.1	77.3	[M-H] ⁻ 1	26297072.1
Isoalantolacton	C15 H20 O2	0.35	232.14641	233.15369	27.371	87.3	80.4	89	[M+H] ⁺ 1	942046426.4

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Pinolenic acid	C18 H30 O2	0.28	278.22466	279.23193	27.881	79.1	60.6	69.4	[M+H] ⁺ 1	7993639.532
Aflatoxin G2	C17 H14 O7	1.14	330.07433	331.0816	27.963			79.4	[M+H] ⁺ 1	1895019.277
Oleanonic acid	C30 H46 O3	-0.36	454.34453	455.35181	28.058	76.2	56.6	81.8	[M+H] ⁺ 1	1406014467
Maslinic acid	C30 H48 O4	-0.43	472.35506	473.36234	28.058	70.1	68	82.8	[M+H] ⁺ 1	61450067.78
9-Oxo-ODE	C18 H30 O3	-0.19	294.21944	295.22672	28.147	89.7	82.2	81.1	[M+H] ⁺ 1	179114493.7
(15Z)-9,12,13-Trihydroxy-15-octadecenoic acid	C18 H34 O5	-0.03	330.24061	329.23334	28.157	81.6	55.3	79.2	[M-H] ⁻ 1	1104429025
Sedanolide	C12 H18 O2	0.54	194.13078	195.13806	28.16	69.2	67.7	71.8	[M+H] ⁺ 1	74223235.5
6-(1,3-Dithiolan-2-yl)-2,2-dimethylchromane	C14 H18 O S2	-3.31	266.07903	267.0863	28.831			70.5	[M+H] ⁺ 1	19265236.74
3-Butylidenephthalide	C12 H12 O2	0.63	188.08385	189.09113	29.087			87	[M+H] ⁺ 1	56990806.78
4-Cyclopentylphenol	C11 H14 O	-0.08	162.10445	161.09717	29.099	77.8	8.9	57.4	[M-H] ⁻ 1	49317744.74
Ligustilide	C12 H14 O2	0.5	190.09947	191.10675	29.283			85.3	[M+H] ⁺ 1	235449595.7

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Formononetin	C16 H12 O4	0.36	268.07366	269.08093	29.357	89.7	9.5	87.9	[M+H] ⁺ 1	6538087.226
Citropten	C11 H10 O4	0.45	206.058	207.06528	29.76	73.2	8.7	73.1	[M+H] ⁺ 1	44177597.54
Resorcinol diglycidyl ether	C12 H14 O4	0.67	222.08936	223.09663	29.954	77	73	60.7	[M+H] ⁺ 1	18184652.49
Mycophenolic acid	C17 H20 O6	0.28	320.12608	343.1153	30.104			73.3	[M+Na] ⁺ 1	8228820.724
Jasmonic acid	C12 H18 O3	0.3	210.12566	211.13293	30.108	80.4	75.5	66.7	[M+H] ⁺ 1	10469168.12
Oxyberberine	C20 H17 N O5	-0.48	351.1105	352.1178	30.617			82.6	[M+H] ⁺ 1	34100171.18
Saikosaponin A	C42 H68 O13	0.67	780.46651	825.46503	30.777			87.3	[M+FA-H] ⁻ 1	259880790.3
Schisandrin	C24 H32 O7	-0.41	432.21463	433.22189	30.986	85.7	9.3	84.8	[M+H] ⁺ 1	187542673.8
Wilforlide A	C30 H46 O3	-0.36	454.34453	455.35181	31.045	67.4	47.6	79.2	[M+H] ⁺ 1	144225276.9
Soyasaponin I	C48 H78 O18	-0.47	942.51837	941.51123	31.082	77.2	8.9	77.2	[M-H] ⁻ 1	7071835.357
Artemisinic acid	C15 H22 O2	0.24	234.16203	235.16931	31.415	85.7	79.3	87.6	[M+H] ⁺ 1	34571604.29
D-(+)-Camphor	C10 H16 O	0.33	152.12016	153.12744	31.596	63.1	65.9	72.2	[M+H] ⁺ 1	28779262.37

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Wogonin	C16 H12 O5	-0.43	284.06835	285.07562	31.653	75.3	8.8	83.4	[M+H] ⁺ 1	34783461.3
Echinocystic acid	C30 H48 O4	0.74	472.35561	473.36288	31.877	65	47.2	82.1	[M+H] ⁺ 1	18101070.03
Nobiletin	C21 H22 O8	0.12	402.13152	403.13879	32.01	92.6	65.1	88.4	[M+H] ⁺ 1	7288693.346
Shogaol	C17 H24 O3	-0.04	276.17253	277.17981	32.03	78.3	49.1	82.5	[M+H] ⁺ 1	16022881.16
5,2'-Dihydroxy- 6,7,8,6'-tetramet hoxyflavone	C19 H18 O8	0.08	374.1002	375.10745	32.063	73.8	53.2	82.6	[M+H] ⁺ 1	54124542.67
Saikosaponin D	C42 H68 O13	0.92	780.46671	825.46503	32.207			86.9	[M+FA-H] ⁻ 1	21404739.96
(-)-Caryophylle ne oxide	C15 H24 O	0.32	220.18279	221.19006	32.366	81.3	76.1	70.8	[M+H] ⁺ 1	16886552.36
Oroxylin A	C16 H12 O5	-0.45	284.06835	285.07562	32.463	76.2	56.6	82.4	[M+H] ⁺ 1	13015214.05
Schisandrin	C24 H32 O7	-0.49	432.21459	433.22189	32.751	84.5	9.2	84.2	[M+H] ⁺ 1	3400926182
Pulchinenoside A	C41 H66 O12	0.16	750.45555	795.4541	33.212			83.1	[M+FA-H] ⁻ 1	342915625.6
Gomisin D	C28 H34 O10	0.52	530.21547	531.22284	33.739	83	51.8	85.1	[M+H] ⁺ 1	59924346.05
α-Hederin	C41 H66 O12	0.24	750.45561	795.4541	33.8			83.2	[M-H] ⁻ 1	258389447.3

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Gomisin J	C22 H28 O6	0.23	388.18868	389.19595	34.097			85.2	[M+H] ⁺ 1	76941462.54
Rutaecarpine	C18 H13 N3 O	0.07	287.10588	288.11316	34.176	66.7	8.3	81.9	[M+H] ⁺ 1	24928907.84
2-Hydroxymyristic acid	C14 H28 O3	-0.14	244.20381	243.19653	34.368	73.9	8.7	53.6	[M-H] ⁻ 1	42290057.14
2-Aminooctadec-4-yne-1,3-diol	C18 H35 N O2	0.38	297.26689	298.27417	34.723	80.2	62	80.7	[M+H] ⁺ 1	50906175.15
(+/-)12(13)-Dihomocercoside	C18 H34 O4	0.58	314.24589	313.23862	35.21	80.1	54.3	84.1	[M-H] ⁻ 1	77318064.14
Phytosphingosine	C18 H39 N O3	0.46	317.29314	318.30042	35.339	75.5	8.8	86.5	[M+H] ⁺ 1	210700608.5
(9Z,12Z)-6,8-Dihydroxy-9,12-octadecadienoic acid	C18 H32 O4	0.77	312.2303	311.22302	35.521	79.6	54	54.8	[M-H] ⁻ 1	69551281.15
(+/-)9,10-dihydroxy-12Z-octadecenoic acid	C18 H34 O4	0.58	314.24589	313.23862	35.624	89.9	60.6	90.9	[M-H] ⁻ 1	125962959.3
Raddeanin A	C47 H76 O16	0.73	896.51399	895.50671	35.668			77.7	[M-H] ⁻ 1	6236922.131
Angeloylgomisin H	C28 H36 O8	-0.1	500.24097	501.24811	35.805	71.4	8.6	72.5	[M+H] ⁺ 1	96210963.65

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Dodemorph	C18 H35 N O	-0.42	281.27175	282.27902	36.64	82.8	51.7		[M+H] ⁺ 1	9495801.629
Atractylenolide II	C15 H20 O2	0.35	232.14641	233.15369	37.519	85.5	79.1	89.1	[M+H] ⁺ 1	64254157.41
Hexadecanedioi c acid	C16 H30 O4	0.5	286.21455	285.20728	37.578	69.9	8.5	76.1	[M-H] ⁻ 1	7051174.545
Dihydrosphingo sine	C18 H39 N O2	0.11	301.29811	302.30539	37.618	72.8	8.6	85	[M+H] ⁺ 1	21655647.88
Dehydrocostus lactone	C15 H18 O2	-0.07	230.13066	231.13794	37.746	90.3	82.5	93.4	[M+H] ⁺ 1	761787328.3
Schisanhenol	C23 H30 O6	0.53	402.20445	403.21173	38.742			85	[M+H] ⁺ 1	890076344.9
Glycerophosph o-N-palmitoyl ethanolamine	C21 H44 N O7 P	0.3	453.28568	454.29282	39.686	70.5	8.5	65	[M+H] ⁺ 1	78674807.5
α-Eleostearic acid	C18 H30 O2	0.06	278.2246	279.23187	39.974	93.3	83.5	92.5	[M+H] ⁺ 1	136910580.4
(R)-3-Hydroxy myristic acid	C14 H28 O3	-0.08	244.20383	243.19655	40.169	65.8	8.3	75.5	[M-H] ⁻ 1	9950868.266
(+/-)9(10)-EpO ME	C18 H32 O3	0.02	296.23515	295.22787	40.534	65.5	46.7	78	[M-H] ⁻ 1	11727901.7
9-Oxo-10(E),12 (E)-octadecadie noic acid	C18 H30 O3	0	294.21949	295.22672	41.947	92.3	83.2	81.9	[M+H] ⁺ 1	67543376.04

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Schizandrin A	C24 H32 O6	-0.06	416.21986	417.22714	43.166			87	[M+H] ⁺ 1	4823209125
α -Cyperone	C15 H22 O	0.72	218.16722	219.1745	43.408	87	80.2	82.3	[M+H] ⁺ 1	13790399.37
Levistilide A	C24 H28 O4	0.29	380.19887	381.20615	43.609			88.8	[M+H] ⁺ 1	67037376.93
Tanshinone IIA	C19 H18 O3	0.49	294.12574	295.13303	43.655	83.9	52.4	82.1	[M+H] ⁺ 1	8514527.763
Schisandrin B	C23 H28 O6	0.19	400.18866	401.19595	44.441			87	[M+H] ⁺ 1	7723793967
Schisandrin C	C22 H24 O6	0.52	384.15749	385.16476	44.976			84	[M+H] ⁺ 1	57557824.99
α -Linolenic acid	C18 H30 O2	0.06	278.2246	279.23187	45.731	86.4	70.6	88.2	[M+H] ⁺ 1	47709923.54
16-Hydroxyhex adecanoic acid	C16 H32 O3	0.58	272.2353	271.22803	45.806	75.3	8.8	77.5	[M-H] ⁻ 1	15702857.66
Oleoyl ethanolamide	C20 H39 N O2	0.67	325.2983	326.30557	45.982	73.5	46.2	69.9	[M+H] ⁺ 1	14120481.82
Glabrolide	C30 H44 O4	0.92	468.32439	469.33163	46.077			71.2	[M+H] ⁺ 1	13888584.1
Erucamide	C22 H43 N O	-0.11	337.33443	338.34171	46.642	90.7	58.6	87.8	[M+H] ⁺ 1	68021204.16
18- β -Glycyrrhet inic acid	C30 H46 O4	0.66	470.33992	469.33264	47.549	73	8.6	71.5	[M-H] ⁻ 1	7617639.593

Name	Formula	Annot.Delta Mass [ppm]	Calc. MW	m/z	RT [min]	mzCloud Best Match	mzCloud Best Match Confidence	mzVault Best Match	Reference Ion	Group Area: PIAO
Stearamide	C18 H37 N O	-0.08	283.28749	284.29477	49.15	89.8	55.8	88.7	[M+H] ⁺ 1	926628513.5
Methamphetam ine	C10 H15 N	0.44	149.12052	150.12779	63.356	71.8	45.3	82.9	[M+H] ⁺ 1	17858115.89

Supplementary Table 4 120 active ingredients of HZJDF

ID	Name	Formula	GI absorption	Lipinski	Ghose	Veber	Egan	Muegge
C1	L-Aspartic acid	C4 H7 N O4	High	Yes	No	Yes	Yes	No
C2	Proline	C5 H9 N O2	High	Yes	No	Yes	Yes	No
C3	Trigonelline	C7 H7 N O2	High	Yes	No	Yes	Yes	No
C4	L-(-)-Malic acid	C4 H6 O5	High	Yes	No	Yes	Yes	No
C5	Fumaric acid	C4 H4 O4	High	Yes	No	Yes	Yes	No
C6	trans-Aconitic acid	C6 H6 O6	High	Yes	No	Yes	Yes	No
C7	Itaconic acid	C5 H6 O4	High	Yes	No	Yes	Yes	No
C8	2-Furoic acid	C5 H4 O3	High	Yes	No	Yes	Yes	No
C9	D-(+)-Pyroglutamic Acid	C5 H7 N O3	High	Yes	No	Yes	Yes	No
C10	Maleic acid	C4 H4 O4	High	Yes	No	Yes	Yes	No
C11	Shikimic acid	C7 H10 O5	High	Yes	No	Yes	Yes	No
C12	Nicotinic acid	C6 H5 N O2	High	Yes	No	Yes	Yes	No
C13	4-Guanidinobutyric acid	C5 H11 N3 O2	High	Yes	No	Yes	Yes	No
C14	Adenine	C5 H5 N5	High	Yes	No	Yes	Yes	No
C15	Guanine	C5 H5 N5 O	High	Yes	No	Yes	Yes	No
C16	Nicotinamide	C6 H6 N2 O	High	Yes	No	Yes	Yes	No
C17	4-Aminophenol	C6 H7 N O	High	Yes	No	Yes	Yes	No
C18	L-Pyroglutamic acid	C5 H7 N O3	High	Yes	No	Yes	Yes	No
C19	Uric acid	C5 H4 N4 O3	High	Yes	No	Yes	Yes	No
C20	L-Norleucine	C6 H13 N O2	High	Yes	No	Yes	Yes	No
C21	L-Tyrosine	C9 H11 N O3	High	Yes	Yes	Yes	Yes	No
C22	Gallic acid	C7 H6 O5	High	Yes	No	Yes	Yes	No
C23	Pyrogallol	C6 H6 O3	High	Yes	No	Yes	Yes	No
C24	L-Phenylalanine	C9 H11 N O2	High	Yes	Yes	Yes	Yes	No

ID	Name	Formula	GI absorption	Lipinski	Ghose	Veber	Egan	Muegge
C25	Maltol	C6 H6 O3	High	Yes	No	Yes	Yes	No
C26	2,3-Dihydroxybenzoic acid	C7 H6 O4	High	Yes	No	Yes	Yes	No
C27	Danshensu	C9 H10 O5	High	Yes	Yes	Yes	Yes	No
C28	Pantothenic acid	C9 H17 N O5	High	Yes	No	Yes	Yes	Yes
C29	Kojic acid	C6 H6 O4	High	Yes	No	Yes	Yes	No
C30	Epigallocatechin (-)	C15 H14 O7	High	Yes	Yes	Yes	Yes	No
C31	Isovanillic acid	C8 H8 O4	High	Yes	Yes	Yes	Yes	No
C32	3,4-Dihydroxyphenylethanol	C8 H10 O3	High	Yes	No	Yes	Yes	No
C33	3-Hydroxybenzyl alcohol	C7 H8 O2	High	Yes	No	Yes	Yes	No
C34	Caffeic acid	C9 H8 O4	High	Yes	Yes	Yes	Yes	No
C35	1,5-Naphthalenediamine	C10 H10 N2	High	Yes	No	Yes	Yes	No
C36	trans-3-Indoleacrylic acid	C11 H9 N O2	High	Yes	Yes	Yes	Yes	No
C37	L-Tryptophan	C11 H12 N2 O2	High	Yes	Yes	Yes	Yes	Yes
C38	Leucylproline	C11 H20 N2 O3	High	Yes	Yes	Yes	Yes	Yes
C39	2,5-Dihydroxybenzaldehyde	C7 H6 O3	High	Yes	No	Yes	Yes	No
C40	Xanthurenic acid	C10 H7 N O4	High	Yes	Yes	Yes	Yes	Yes
C41	4-Phenylbutyric acid	C10 H12 O2	High	Yes	Yes	Yes	Yes	No
C42	Indole-3-carboxaldehyde	C9 H7 N O	High	Yes	No	Yes	Yes	No
C43	2-Isopropylmalic acid	C7 H12 O5	High	Yes	Yes	Yes	Yes	No
C44	Esculetin	C9 H6 O4	High	Yes	No	Yes	Yes	No
C45	1-Naphthol	C10 H8 O	High	Yes	No	Yes	Yes	No
C46	Methyl gallate	C8 H8 O5	High	Yes	Yes	Yes	Yes	No
C47	Isoferulic acid	C10 H10 O4	High	Yes	Yes	Yes	Yes	No
C48	BMK methyl glycidate	C11 H12 O3	High	Yes	Yes	Yes	Yes	No
C49	Terephthalic acid	C8 H6 O4	High	Yes	No	Yes	Yes	No

ID	Name	Formula	GI absorption	Lipinski	Ghose	Veber	Egan	Muegge
C50	Benzoic acid	C7 H6 O2	High	Yes	No	Yes	Yes	No
C51	4-Coumaric acid	C9 H8 O3	High	Yes	Yes	Yes	Yes	No
C52	Catechin	C15 H14 O6	High	Yes	Yes	Yes	Yes	Yes
C53	2,3,4,9-Tetrahydro-1H- β -carboline-3-carboxylic acid	C12 H12 N2 O2	High	Yes	Yes	Yes	Yes	Yes
C54	(-)-Gallocatechin	C15 H14 O7	High	Yes	Yes	Yes	Yes	No
C55	4-Hydroxymandelic acid	C8 H8 O4	High	Yes	Yes	Yes	Yes	No
C56	Fraxetin	C10 H8 O5	High	Yes	Yes	Yes	Yes	Yes
C57	6,7-Dihydroxycoumarin	C9 H6 O4	High	Yes	No	Yes	Yes	No
C58	5-Hydroxymethylfurfural	C6 H6 O3	High	Yes	No	Yes	Yes	No
C59	Ferulic acid	C10 H10 O4	High	Yes	Yes	Yes	Yes	No
C60	Acetophenone	C8 H8 O	High	Yes	No	Yes	Yes	No
C61	Taxifolin	C15 H12 O7	High	Yes	Yes	Yes	Yes	Yes
C62	(+)-Magnoflorine	C20 H23 N O4	High	Yes	Yes	Yes	Yes	Yes
C63	Syringic acid	C9 H10 O5	High	Yes	Yes	Yes	Yes	No
C64	2,4-Dimethylbenzaldehyde	C9 H10 O	High	Yes	No	Yes	Yes	No
C65	N-Acetyl-L-phenylalanine	C11 H13 N O3	High	Yes	Yes	Yes	Yes	Yes
C66	Vanillin	C8 H8 O3	High	Yes	No	Yes	Yes	No
C67	3-Phenyllactic acid	C9 H10 O3	High	Yes	Yes	Yes	Yes	No
C68	Quercetin	C15 H10 O7	High	Yes	Yes	Yes	Yes	Yes
C69	Scopoletin	C10 H8 O4	High	Yes	Yes	Yes	Yes	No
C70	Ellagic acid	C14 H6 O8	High	Yes	Yes	No	No	Yes
C71	Yohimbine	C21 H26 N2 O3	High	Yes	Yes	Yes	Yes	Yes
C72	Isofraxidin	C11 H10 O5	High	Yes	Yes	Yes	Yes	Yes
C73	(+)-Pinoresinol	C20 H22 O6	High	Yes	Yes	Yes	Yes	Yes

ID	Name	Formula	GI absorption	Lipinski	Ghose	Veber	Egan	Muegge
C74	Demethyleneberberine	C19 H17 N O4	High	Yes	Yes	Yes	Yes	Yes
C75	Berberrubine	C19 H15 N O4	High	Yes	Yes	Yes	Yes	Yes
C76	Kaempferol	C15 H10 O6	High	Yes	Yes	Yes	Yes	Yes
C77	trans-Cinnamaldehyde	C9 H8 O	High	Yes	No	Yes	Yes	No
C78	Azelaic acid	C9 H16 O4	High	Yes	Yes	Yes	Yes	No
C79	Salicylic acid	C7 H6 O3	High	Yes	No	Yes	Yes	No
C80	Jatrorrhizine	C20 H19 N O4	High	Yes	Yes	Yes	Yes	Yes
C81	5,7,8-Trihydroxyflavone	C15 H10 O5	High	Yes	Yes	Yes	Yes	Yes
C82	Scoparone	C11 H10 O4	High	Yes	Yes	Yes	Yes	Yes
C83	Parthenolide	C15 H20 O3	High	Yes	Yes	Yes	Yes	Yes
C84	Phenylacetaldehyde	C8 H8 O	High	Yes	No	Yes	Yes	No
C85	Palmatine	C21 H21 N O4	High	Yes	Yes	Yes	Yes	Yes
C86	Liquiritigenin	C15 H12 O4	High	Yes	Yes	Yes	Yes	Yes
C87	Berberine	C20 H17 N O4	High	Yes	Yes	Yes	Yes	Yes
C88	Luteolin	C15 H10 O6	High	Yes	Yes	Yes	Yes	Yes
C89	Dehydrocorydaline	C22 H23 N O4	High	Yes	Yes	Yes	Yes	Yes
C90	Phloretin	C15 H14 O5	High	Yes	Yes	Yes	Yes	Yes
C91	9S,13R-12-Oxophytodienoic acid	C18 H28 O3	High	Yes	Yes	No	Yes	Yes
C92	Corchorifatty acid F	C18 H32 O5	High	Yes	Yes	No	Yes	Yes
C93	Matairesinol	C20 H22 O6	High	Yes	Yes	Yes	Yes	Yes
C94	Isoalantolactone	C15 H20 O2	High	Yes	Yes	Yes	Yes	Yes
C95	3-Butylidenephthalide	C12 H12 O2	High	Yes	Yes	Yes	Yes	No
C96	Ligustilide	C12 H14 O2	High	Yes	Yes	Yes	Yes	No
C97	Formononetin	C16 H12 O4	High	Yes	Yes	Yes	Yes	Yes
C98	Oxyberberine	C20 H17 N O5	High	Yes	Yes	Yes	Yes	Yes

ID	Name	Formula	GI absorption	Lipinski	Ghose	Veber	Egan	Muegge
C99	Schisandrin	C24 H32 O7	High	Yes	Yes	Yes	Yes	Yes
C100	Artemisinic acid	C15 H22 O2	High	Yes	Yes	Yes	Yes	Yes
C101	Wogonin	C16 H12 O5	High	Yes	Yes	Yes	Yes	Yes
C102	Nobiletin	C21 H22 O8	High	Yes	Yes	Yes	Yes	Yes
C103	Shogaol	C17 H24 O3	High	Yes	Yes	Yes	Yes	Yes
C104	5,2'-Dihydroxy-6,7,8,6'-tetramethoxyflavone	C19 H18 O8	High	Yes	Yes	Yes	Yes	Yes
C105	Oroxylin A	C16 H12 O5	High	Yes	Yes	Yes	Yes	Yes
C106	Gomisin J	C22 H28 O6	High	Yes	Yes	Yes	Yes	Yes
C107	Rutaecarpine	C18 H13 N3 O	High	Yes	Yes	Yes	Yes	Yes
C108	2-Aminooctadec-4-yne-1,3-diol	C18 H35 N O2	High	Yes	Yes	No	Yes	No
C109	(+/-)12(13)-DiHOME	C18 H34 O4	High	Yes	Yes	No	Yes	Yes
C110	(+/-)9,10-dihydroxy-12Z-octadecenoic acid	C18 H34 O4	High	Yes	Yes	No	Yes	Yes
C111	Atractylenolide II	C15 H20 O2	High	Yes	Yes	Yes	Yes	Yes
C112	Dehydrocostus lactone	C15 H18 O2	High	Yes	Yes	Yes	Yes	Yes
C113	Schisanhenol	C23 H30 O6	High	Yes	Yes	Yes	Yes	Yes
C114	α -Eleostearic acid	C18 H30 O2	High	Yes	No	No	Yes	No
C115	9-Oxo-10(E),12(E)-octadecadienoic acid	C18 H30 O3	High	Yes	Yes	No	Yes	No
C116	α -Cyperone	C15 H22 O	High	Yes	Yes	Yes	Yes	No
C117	Tanshinone IIA	C19 H18 O3	High	Yes	Yes	Yes	Yes	Yes
C118	Schisandrin B	C23 H28 O6	High	Yes	Yes	Yes	Yes	No
C119	Schisandrin C	C22 H24 O6	High	Yes	Yes	Yes	Yes	Yes
C120	Methamphetamine	C10 H15 N	High	Yes	No	Yes	Yes	No

Supplementary Table 5 640 intersection targets between HZJDF and CAC

NO.	Target name
1	EGLN1
2	ADORA3
3	GRM3
4	HDAC3
5	CACNA2D1
6	PEPD
7	KDM6B
8	KDM5C
9	SLC1A1
10	ACLY
11	PLG
12	FNTA
13	FNTB
14	ACE
15	REN
16	ANPEP
17	F2
18	NR1H4
19	PLA2G2A
20	NOS1
21	NOS2
22	NOS3
23	MME
24	DPP4

25	XIAP
26	LAP3
27	ODC1
28	HSD11B1
29	HLA-A
30	ACE2
31	PTGS2
32	CTSB
33	CA2
34	CA1
35	CA9
36	EPHX2
37	CNR1
38	PRKCA
39	SIRT2
40	FAP
41	CTSL
42	PLA2G4A
43	PLA2G1B
44	CNR2
45	CTSD
46	NTSR1
47	FPR2
48	ENPEP
49	CFB
50	SI

51	AR
52	CHRNA7
53	CHRNA7
54	ITGB3
55	HCAR2
56	MMP9
57	MMP2
58	IMPDH2
59	PTPN1
60	P4HTM
61	MMP3
62	MMP1
63	PLK1
64	CYP2A6
65	KDM4D
66	PARP1
67	PIM3
68	NR4A1
69	EGLN3
70	FAAH
71	CYP19A1
72	MMP8
73	CCR2
74	HDAC1
75	IKBKB
76	KIT

77	PDGFRA
78	FGFR3
79	FGFR1
80	ERN1
81	AKR1B1
82	CYP11B1
83	CYP3A4
84	CYP17A1
85	RAF1
86	EPHX1
87	JAK2
88	CHEK1
89	CHAT
90	DHFR
91	CYP51A1
92	ACHE
93	PTPN2
94	TNF
95	KDM3A
96	FTO
97	EGLN2
98	KDM5B
99	CSNK2A1
100	FYN
101	LCK
102	ESR2

103	HSP90AA1
104	HDAC6
105	HDAC4
106	SLC6A4
107	ITGAL
108	PTGER1
109	PTGER4
110	PTGFR
111	PTGER3
112	RORA
113	FDFT1
114	NR3C1
115	PTGER2
116	PTGIR
117	PPARG
118	PPARA
119	PPARD
120	POLB
121	LTB4R
122	IDO1
123	NR3C2
124	HSD11B2
125	STAT3
126	ALOX5
127	TRPV4
128	PRKCH

129	PTPN11
130	AKR1B10
131	PGR
132	BCHE
133	PTGES
134	NR1H3
135	DNTT
136	ESR1
137	GSTM1
138	PRKCD
139	CDC25A
140	POLA1
141	PRKCB
142	PRKCQ
143	G6PD
144	IL6
145	ADAM17
146	GLUL
147	GPBAR1
148	FABP1
149	VAV1
150	ATP12A
151	RORC
152	CD81
153	MAPK3
154	ACP1

155	ABCB1
156	VDR
157	PCSK7
158	TLR4
159	FEN1
160	TOP2A
161	HDAC2
162	SGK1
163	PTGS1
164	MDH2
165	DYRK1A
166	MIF
167	CCR1
168	ADORA2A
169	GPR35
170	HTR2B
171	TYMP
172	FBP1
173	PNP
174	PLAU
175	SLC15A1
176	ARG1
177	TYMS
178	CCNE1
179	ADORA2B
180	ADA

181	CDK2
182	PTK2B
183	AKT2
184	TLR9
185	MGMT
186	ABL1
187	AKT1
188	AURKA
189	PRKD2
190	BRAF
191	EPHB2
192	VCAM1
193	KAT2B
194	CCNB1
195	CDK1
196	MAPK8
197	MAPK9
198	KDR
199	MAPK10
200	ALOX15
201	CTNNB1
202	TAAR1
203	HPRT1
204	ERBB2
205	CES1
206	GABRA5

207	CDK9
208	KCNN3
209	CDK5
210	CCNA2
211	CDK4
212	GSK3B
213	ELANE
214	FPR1
215	AAK1
216	MGLL
217	NAMPT
218	PADI2
219	PADI4
220	PIK3CD
221	PIK3CB
222	PIK3CG
223	PIK3CA
224	USP7
225	GAK
226	MAP3K14
227	GSK3A
228	EP300
229	MAP2K1
230	MCL1
231	PTPRC
232	DUSP1

233	ICAM1
234	SELE
235	MAPK1
236	DNMT1
237	ADH1B
238	DNMT3A
239	CFTR
240	SIRT1
241	TGM2
242	PTPN22
243	TRPV1
244	AOC3
245	ALDH2
246	ALDH1A1
247	SCD
248	CHUK
249	MMP12
250	NUDT1
251	IGF1R
252	CSF1R
253	DRD2
254	PSMB8
255	SNCA
256	TYR
257	JAK3
258	DAPK3

259	DAPK2
260	PLK4
261	RPS6KA2
262	TTK
263	CLK2
264	STK17A
265	MAPK12
266	CSNK1E
267	EPHA3
268	EIF2AK2
269	STK3
270	MAP2
271	XDH
272	RPS6KA3
273	CA4
274	EGFR
275	SRC
276	UPP1
277	CASP8
278	PTGDR2
279	NRP1
280	FURIN
281	HGFAC
282	GZMB
283	BRD4
284	BRD2

285	BRDT
286	PDE4A
287	DPYD
288	EDNRA
289	ADRA1B
290	OPRM1
291	GSR
292	CHEK2
293	PLAUR
294	NGF
295	NOD1
296	NOD2
297	FABP5
298	FABP2
299	TH
300	SLC7A5
301	SPHK1
302	TBXAS1
303	CDC25C
304	APEX1
305	PTPRA
306	MAPKAPK2
307	GRB2
308	MTNR1A
309	TACR1
310	CTBP2

311	PCNA
312	HTR3A
313	MMP13
314	CASR
315	ITGB1
316	ITGA5
317	MTNR1B
318	MGAM
319	CYP1A2
320	CCR3
321	FUT7
322	LDHA
323	ALK
324	SERPINE1
325	BCL2L1
326	TPMT
327	AKR1C3
328	ALB
329	PTK2
330	MET
331	AXL
332	AKR1C1
333	FASN
334	RARG
335	RARB
336	DYRK1B

337	CRHR1
338	BCL2
339	SLC29A1
340	RXRB
341	RXRA
342	DBH
343	NQO1
344	FFAR4
345	CXCL8
346	S1PR2
347	S1PR1
348	CYP26B1
349	ABCG2
350	CASP3
351	MB
352	ST6GAL1
353	CYP1B1
354	ABCC1
355	AHR
356	EPAS1
357	TNKS
358	CISD1
359	CASP4
360	CASP9
361	CASP6
362	CASP7

363	CDK6
364	ALOX12
365	CYP1A1
366	TACR2
367	PRKDC
368	OGA
369	MPO
370	AMPD3
371	ITGB2
372	PDCD4
373	JUN
374	NGFR
375	OTC
376	CXCR2
377	DNMT3B
378	PLA2G10
379	HMGCR
380	SELL
381	SELP
382	GRK6
383	CPT1A
384	PARP10
385	PDGFRB
386	GSTP1
387	PYGM
388	ILK

389	CASP1
390	AMPD2
391	HSPA5
392	GAPDH
393	HSPA8
394	TERT
395	CASP2
396	LIG1
397	PFKFB3
398	PRKACA
399	GGH
400	RARA
401	TRPM8
402	SLC16A1
403	TRPA1
404	CMA1
405	PIK3R1
406	HRH4
407	PKM
408	CHRM3
409	CTSG
410	SYK
411	CYP2C9
412	CYP2C19
413	F3
414	NFE2L2

415	RELA
416	CCND1
417	CYP2D6
418	ATP4A
419	P2RX7
420	MAP2K2
421	PARP2
422	ALPL
423	HSPA1A
424	SLC16A3
425	CSNK2A2
426	KIF20A
427	TAS1R3
428	MC1R
429	PDPK1
430	EPHA2
431	EPHB3
432	EPHB4
433	EPHA1
434	CTSC
435	EDNRB
436	GHSR
437	CCKBR
438	RAD51
439	TNFRSF10A
440	BIRC3

441	BIRC2
442	CTSE
443	ADAM9
444	FOS
445	WDR5
446	HRH1
447	WEE1
448	NAT1
449	VCP
450	MPG
451	GSTA1
452	MANBA
453	UGCG
454	SHH
455	PRSS1
456	NR1H2
457	TPO
458	MALT1
459	ADH1C
460	HMOX1
461	CCR5
462	CCR8
463	FLT4
464	INSR
465	TEK
466	MAP3K8

467	LYN
468	CBR1
469	KCNA3
470	NFKB1
471	PON1
472	CXCR1
473	TOP1
474	JAK1
475	ASAH1
476	FADS1
477	NEK6
478	SLC37A4
479	IKBKG
480	IGFBP3
481	SOAT1
482	SLC11A2
483	FLT1
484	ADAMTS4
485	MAPK14
486	MTOR
487	ROCK1
488	RPS6KB1
489	F13A1
490	IDH1
491	SLC9A1
492	PLA2G2D

493	PLA2G7
494	PHLPP2
495	PRMT1
496	PLCG1
497	SSTR5
498	SSTR2
499	ITGAV
500	CREBBP
501	RHOA
502	PPP5C
503	HNF4A
504	ITGA1
505	KCNN4
506	HCK
507	PI4KB
508	CSNK1A1
509	RET
510	DYRK2
511	MAPT
512	ST14
513	GLI1
514	PTPN6
515	CDK8
516	PRKD1
517	HDAC7
518	DAPK1

519	MYLK
520	PTPRS
521	CD38
522	GPR55
523	SMYD2
524	NR1I2
525	IRAK1
526	IRAK4
527	PRSS3
528	HIF1A
529	WNT3A
530	TGFBR2
531	TGFBR1
532	MAP3K5
533	PIK3C3
534	ENPP2
535	MDM4
536	F12
537	EIF2AK3
538	BDKRB1
539	PRF1
540	MMP7
541	CDC42
542	RAC1
543	HPGD
544	MMP14

545	GRIN2B
546	NCOR2
547	NCOR1
548	HDAC9
549	BMP4
550	ROCK2
551	PNMT
552	LIMK2
553	MAP2K3
554	BTK
555	PBK
556	NTRK3
557	TYK2
558	PTPN13
559	NLRP3
560	SLC2A1
561	MDM2
562	CTSF
563	HRH2
564	PGK1
565	NTRK1
566	MST1R
567	VEGFA
568	XBP1
569	ATR
570	SFRP1

571	GUSB
572	MMP26
573	STAT1
574	RBP4
575	GART
576	KEAP1
577	ITGB5
578	ITGB6
579	PRKCZ
580	QPCTL
581	YES1
582	BLK
583	CSK
584	XPO1
585	PLA2G6
586	HSP90AB1
587	HTT
588	TSPO
589	IL2
590	EZR
591	BAD
592	BIRC5
593	CX3CR1
594	TLR7
595	TLR8
596	SREBF2

597	HSP90B1
598	MT-ND4
599	SMARCA4
600	NOX1
601	EHMT2
602	MAP3K11
603	CCR9
604	TNFRSF1A
605	BDKRB2
606	SPHK2
607	LPAR2
608	EZH2
609	TNK2
610	MAP3K7
611	TPH1
612	TAB1
613	SGPL1
614	PAK1
615	IL1B
616	F2RL1
617	UTS2R
618	STK17B
619	LDLR
620	ATM
621	USP47
622	PTGES2

623	TP53
624	GCG
625	PRKAA2
626	PRKAB1
627	CENPE
628	SCN2A
629	EED
630	SUZ12
631	C5AR1
632	PPOX
633	ERBB4
634	TGFB1
635	SLC22A2
636	CARM1
637	CXCR3
638	S100B
639	PTPRCAP
640	ITGA4
