

The detailed information on chemical composition of KHJSC

ID	chemical composition	m/z	RT	Model	Formula	Mass Error (ppm)
1	Oxalic acid	202.98	0.48	pos	C2H2O4	0.12
2	Betaine	118.09	0.69	pos	C5H11NO2	-0.68
3	D-Digitoxose	190.11	0.73	pos	C6H12O4	-3.37
4	Isoguvacine	110.06	0.74	pos	C6H9NO2	0.67
5	Cytisine	191.12	0.75	pos	C11H14N2O	-2.32
6	Aconitic acid	175.02	1.10	pos	C6H6O6	-2.11
7	Swainsonine	174.11	1.34	pos	C8H15NO3	-2.08
8	Ecgonine Methyl Ester	200.13	1.47	pos	C10H17NO3	-2.16
9	Lupinine	170.15	1.64	pos	C10H19NO	-2.48
10	Vanillylamine	136.08	1.80	pos	C8H11NO2	-1.58
11	Matrine	249.20	1.82	pos	C15H24N2O	-2.62
12	Vidarabine	268.10	1.99	pos	C10H13N5O4	-1.62
13	Sophocarpine	493.35	2.00	pos	C15H22N2O	-3.00
14	Protoanemonin	193.05	2.03	pos	C5H4O2	-2.29
15	P-Coumaric Acid	147.04	2.03	pos	C9H8O3	-2.02
16	Lupanine	497.38	2.19	pos	C15H24N2O	-2.55
17	Dolichosterone	495.37	2.24	pos	C28H46O5	0.33
18	Syringic Acid	199.06	2.24	pos	C9H10O5	-2.48
19	Maltol	275.05	2.28	pos	C6H6O3	7.83
20	Vincamine	355.20	2.62	pos	C21H26N2O3	-3.24
21	Licoagroside B	433.13	2.68	pos	C18H24O12	-2.52
22	Phaseolotoxin	499.20	2.72	pos	C14H33N10O7PS	-0.67
23	Mangiferin	455.11	2.79	pos	C19H18O11	-8.73
24	Pisumionoside	437.23	2.93	pos	C19H32O9	-8.67
25	Asperulosidic acid	455.11	3.16	pos	C18H24O12	-3.14
26	Naringin	563.17	3.25	pos	C27H32O14	-2.58
27	Gentisyl Alcohol	141.05	3.26	pos	C7H8O3	-2.33
28	Puerarin	417.12	3.28	pos	C21H20O9	-3.05
29	Z-Clausenamide	600.29	3.40	pos	C18H17NO2	4.15
30	Chrysophanol 1-triglucoside	741.22	3.45	pos	C33H40O19	-2.94
31	Ginsenoside Rh4	333.21	3.47	pos	C36H60O8	7.51
32	Pimpinellin	247.06	3.57	pos	C13H10O5	-2.75
33	Dehydromonocrotaline	387.15	3.70	pos	C16H21NO6	3.95
34	Wogonin	285.07	3.72	pos	C16H12O5	-2.86
35	Trifolirhizin	447.13	3.73	pos	C22H22O10	-2.77
36	Lycoperoside D	740.46	3.84	pos	C39H65NO12	5.27
37	Isomangiferin	455.11	3.84	pos	C19H18O11	-8.62
38	Isoeriocitrin	579.17	4.08	pos	C27H32O15	-2.54
39	Sakuranetin	328.12	4.16	pos	C16H14O5	-3.56
40	Notoginsenoside Fe	470.27	4.16	pos	C47H80O17	6.75
41	Omphalotin C	773.96	4.55	pos	C76H125N13O19	-0.08
42	Narirutin	563.17	4.67	pos	C27H32O14	-2.59
43	Rutarin	447.13	4.73	pos	C20H24O10	2.87
44	Ononin	431.13	4.81	pos	C22H22O9	-2.80
45	Cimicifugoside	692.40	4.91	pos	C37H54O11	5.50
46	Glycitin	464.15	5.08	pos	C22H22O10	-2.57
47	Piperonal	151.04	5.10	pos	C8H6O3	-2.09
48	P-Anisaldehyde	137.06	5.27	pos	C8H8O2	-1.85
49	Coumarin	147.04	5.28	pos	C9H6O2	-2.85
50	Cirsimaritin	315.09	5.34	pos	C17H14O6	-3.33
51	Gentisate aldehyde	299.05	5.52	pos	C7H6O3	6.02

52	Brucein E	377.16	5.56	pos	C20H28O9	-2.34
53	Madlongiside C	650.39	5.57	pos	C35H56O10	-7.68
54	Glycyrrhetic Acid	471.35	5.58	pos	C30H46O4	-2.08
55	Genistein	271.06	5.58	pos	C15H10O5	-2.35
56	3,7-Dimethylquercetin	313.07	5.60	pos	C17H14O7	-2.25
57	Lactucin	299.09	5.62	pos	C15H16O5	6.02
58	Kaempferide	283.06	5.64	pos	C16H12O6	-2.43
59	Nobiletin	403.14	5.66	pos	C21H22O8	-2.55
60	Tangeritin	373.13	5.71	pos	C20H20O7	-2.69
61	Chavicol	135.08	5.74	pos	C9H10O	-1.55
62	Calycosin	285.07	6.01	pos	C16H12O5	-3.19
63	Violet-leaf aldehyde	121.10	6.14	pos	C9H14O	-0.65
64	Daidzein	255.06	6.32	pos	C15H10O4	-3.21
65	Hesperetin	285.08	7.37	pos	C16H14O6	-2.45
66	Torachryson	269.08	7.38	pos	C14H14O4	6.73
67	Umbelliferone	163.04	7.97	pos	C9H6O3	-2.46
ID	chemical composition	m/z	RT	Model	Formula	Mass Error (ppm)
68	Neohesperidose	371.12	0.60	neg	C12H22O10	-1.07
69	Hesperidin	609.19	0.65	neg	C28H34O15	8.88
70	Trans-Aconitic Acid	173.01	0.73	neg	C6H6O6	-4.39
71	Cis-Aconitic anhydride	155.00	0.74	neg	C6H4O5	-5.48
72	Gallic Acid	169.01	1.78	neg	C7H6O5	-4.71
73	Gentisic Acid	153.02	2.36	neg	C7H6O4	-5.55
74	Tuliposide B	315.07	2.45	neg	C11H18O9	7.23
75	Paeonol	165.05	2.56	neg	C9H10O3	-5.10
76	4-Coumaryl alcohol	149.06	2.60	neg	C9H10O2	-5.98
77	Theogallin	343.07	2.70	neg	C14H16O10	-1.17
78	Coumarinic acid	209.05	2.74	neg	C9H8O3	-3.26
79	Osmundalactone	109.03	2.77	neg	C6H8O3	-7.89
80	Isocoumarin	181.01	2.94	neg	C9H6O2	-4.46
81	Fraxetin	207.03	3.02	neg	C10H8O5	-2.96
82	Bergenin	363.05	3.02	neg	C14H16O9	-0.75
83	Valtrate	193.05	3.05	neg	C10H12O5	-3.22
84	Troxerutin	723.21	3.16	neg	C33H42O19	-0.80
85	Isoferulic acid	239.06	3.44	neg	C10H10O4	-2.22
86	Quercetin 3-sulfate	427.00	3.48	neg	C15H10O10S	-2.37
87	Homovanillin	165.05	3.60	neg	C9H10O3	-4.90
88	Cinnamoside	517.23	3.66	neg	C24H38O12	-0.96
89	Noreugenin	191.03	3.73	neg	C10H8O4	-3.34
90	Neoisostilbin	449.11	3.80	neg	C21H22O11	-1.37
91	Cis-Aconitic acid	173.01	3.81	neg	C6H6O6	-4.28
92	Daidzin	397.09	3.86	neg	C21H20O9	-1.37
93	Chrysophanein	461.11	3.99	neg	C21H20O9	-0.06
94	Vanillin	151.04	4.04	neg	C8H8O3	-5.73
95	Quercetin 7-xyloside	479.08	4.06	neg	C20H18O11	-1.14
96	Scopoletin	237.04	4.10	neg	C10H8O4	-1.61
97	Sarmentosin	312.05	4.13	neg	C11H17NO7	-2.43
98	Bengenin	327.07	4.14	neg	C14H16O9	-1.03
99	Uralennoiside	285.06	4.18	neg	C12H14O8	-1.10
100	Isoorientin	493.10	4.19	neg	C21H20O11	-0.66
101	Sinapic Acid	223.06	4.21	neg	C11H12O5	-2.38
102	Acacetin	283.06	4.22	neg	C16H12O5	-1.09
103	Physcion 8-glucoside	445.11	4.41	neg	C22H22O10	-0.44
104	Syringaresinol	417.15	4.43	neg	C22H26O8	-1.64

105	Quercetin 7-glucoside	463.09	4.50	neg	C21H20O12	-0.34
106	Acacetin 7	577.16	4.50	neg	C27H30O14	-0.72
107	Genistein 7-O-Glucoside	431.10	4.53	neg	C21H20O10	-0.91
108	Nodakenin	453.14	4.54	neg	C20H24O9	-0.30
109	Phloretin	273.08	5.17	neg	C15H14O5	-0.68
110	Mellein	223.06	5.17	neg	C10H10O3	-2.99
111	Formononetin-7-O-Glucoside	475.12	5.24	neg	C22H22O9	-1.49
112	Formononetin	267.07	5.24	neg	C16H12O4	-1.09
113	Coumafuryl	297.08	5.42	neg	C17H14O5	-1.77
114	Astilbin	449.11	5.42	neg	C21H22O11	-0.67
115	Esculetin	177.02	5.43	neg	C9H6O4	-4.23
116	Wistin	505.14	5.45	neg	C23H24O10	-0.26
117	Phaseolic acid	243.12	5.46	neg	C12H22O6	-1.41
118	Prunetinoside	491.12	5.47	neg	C22H22O10	-1.05
119	Isoliquiritigenin	255.07	5.51	neg	C15H12O4	-1.14
120	Biochanin A	283.06	5.55	neg	C16H12O5	-1.13
121	Eugenin	251.06	5.56	neg	C11H10O4	-1.76
122	Alizarin	285.04	5.56	neg	C14H8O4	-1.13
123	Cucurbitic acid	257.14	5.59	neg	C12H20O3	-1.31
124	Capsianoside I	659.33	5.59	neg	C32H52O14	-0.52
125	Patuletin	313.04	5.59	neg	C16H12O8	-0.69
126	Pinoquercetin	297.04	5.60	neg	C16H12O7	-1.04
127	Isostevioside	803.37	5.64	neg	C38H60O18	-0.54
128	RUBUSOSIDE	641.32	5.65	neg	C32H50O13	-0.99
129	Quercetin	301.04	5.67	neg	C15H10O7	-1.01
130	Dulcoside A	787.38	5.67	neg	C38H60O17	-0.40
131	Pseudobaptigenin	281.05	5.67	neg	C16H10O5	-1.18
132	Tectochrysin	267.07	5.67	neg	C16H12O4	-0.93
133	REBAUDIOSIDE C	949.43	5.68	neg	C44H70O22	-0.72
134	Steviobioside	687.32	5.71	neg	C32H50O13	-0.87
135	Neoandrographolide	525.27	5.74	neg	C26H40O8	-2.15
136	Geranic acid	213.11	5.89	neg	C10H16O2	-3.40
137	Isorhamnetin	297.04	5.98	neg	C16H12O7	-1.35
138	Isosakuranetin	267.07	6.25	neg	C16H14O5	-0.98
139	Isoimperatorin	269.08	6.25	neg	C16H14O4	-0.96
140	Scoparone	251.06	6.25	neg	C11H10O4	-2.39
141	Glycitein	283.06	7.15	neg	C16H12O5	-0.81
142	Marmesin	267.07	7.16	neg	C14H14O4	8.60
143	Stevioside	803.37	7.16	neg	C38H60O18	-0.45