

1 **Supplementary Material**

2 Nontargeted metabolomics coupled with multivariate modelling
3 techniques for discrimination of *Cyclocarya paliurus* (Batal.)
4 Ijinskaja leaves from different geographic altitudes

5 Yuhao Li^a, Huiting Xi^a, Lei Feng^a, Lu Liang^b, Tianming Yang^b,

6 Xuejin Mao^{a,b}, Yuanxing Wang^{*,a,b}

7 ^a State Key Laboratory of Food Science and Technology, Nanchang University,

8 Nanchang 330047, China

9 ^b College of Food Science, Nanchang University, Jiangxi, China

10 *Corresponding author: Dr. Yuanxing Wang

11 Telephone: +86-0791-88304400

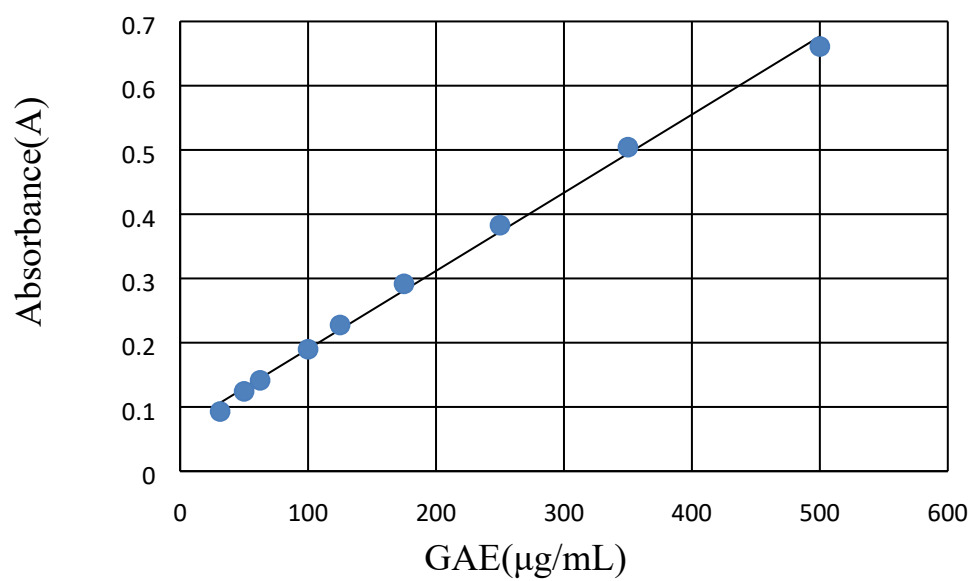
12 Email: yuanxingwang@ncu.edu.cn (Yuanxing Wang)

13 The lists of Supplementary Material

- 14 ● The standard curves of the TPC and TFC (Fig. S1).
- 15 ● The TIC diagram in the negative modes for five different altitude environments of *C.*
16 *paliurus* leaves (Fig. S2).
- 17 ● The MS/MS information of all identified compounds (Fig. S3).
- 18 ● Heatmap of 70 compounds (Fig. S4)
- 19 ● QC sample were clustered in the center of the PCA plot (Fig. S5).
- 20 ● Cluster dendrogram of the data set concluded for five different altitude
21 environments of *C. paliurus* leaves (Fig. S6).
- 22 ● Variable importance on projection (VIP) scores from the PLS-DA model indicating
23 the most discriminating metabolites among *C. paliurus* leaves from different altitude
24 environments in descending order of importance with relative levels of the metabolite
25 (Fig. S7).
- 26 ● Correlation analysis heatmap of fifteen metabolites with $VIP > 1.0$ and $P < 0.05$ (* $P <$
27 0.05 , ** $P < 0.01$, *** $P < 0.001$). (Fig. S8).
- 28 ● Pathway topology analysis related with differential metabolites (Fig. S9).
- 29 ● The information concerning the identification of 70 compounds (Table S1).

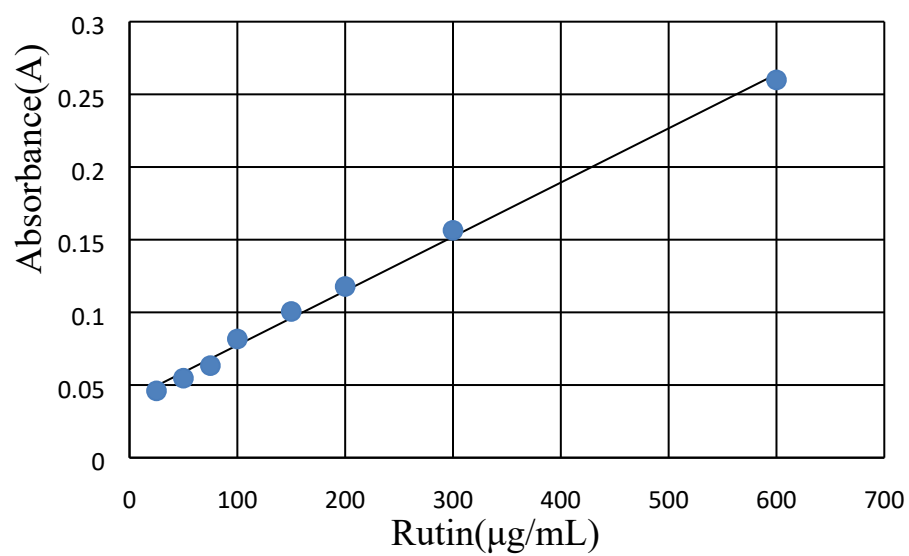
30 ● The standard curves of the TPC and TFC (Fig. S1).

31 TPC



32

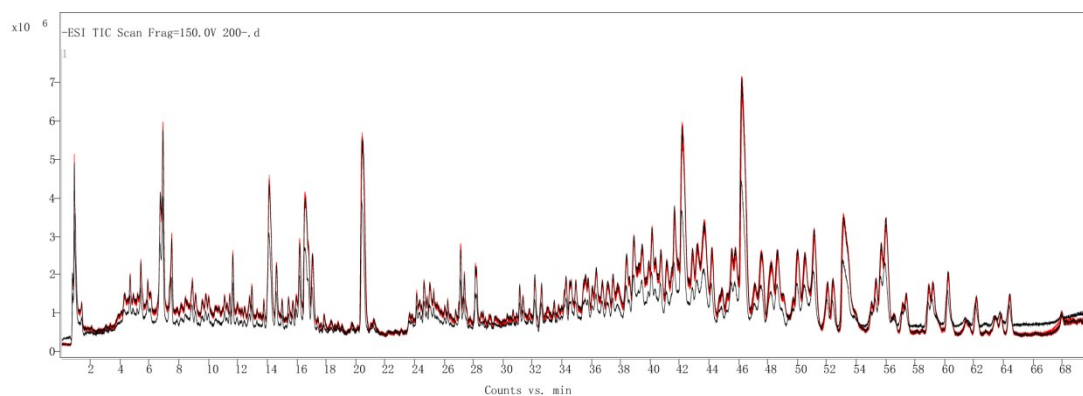
33 TFC



34

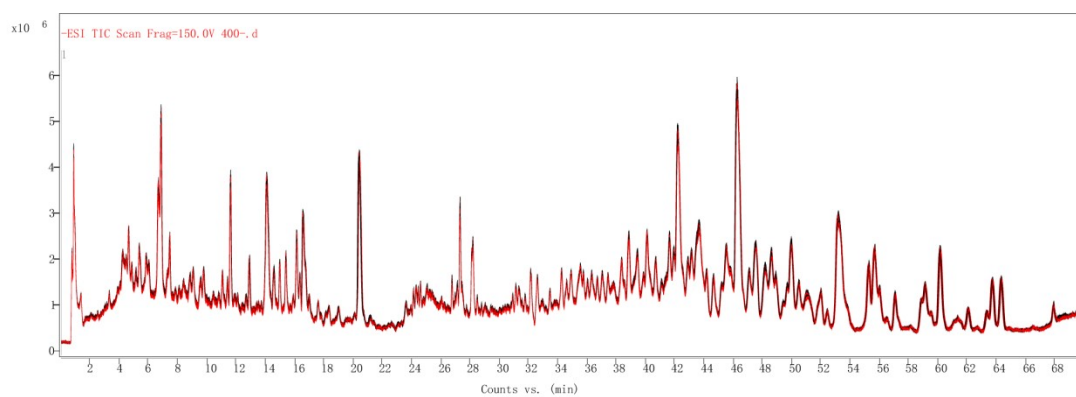
35 ● The TIC diagram in the negative modes for five different altitude environments of *C.*
36 *paliurus* leaves (Fig. S2).

37 200 m



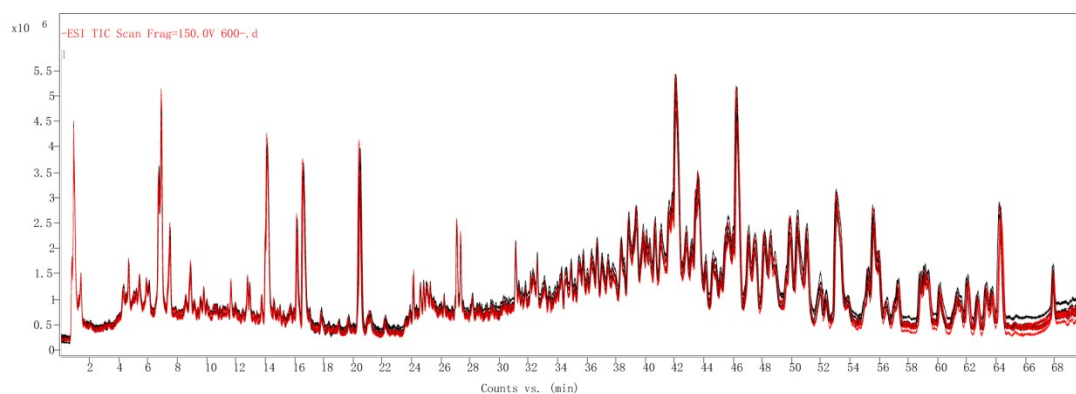
38

39 400 m



40

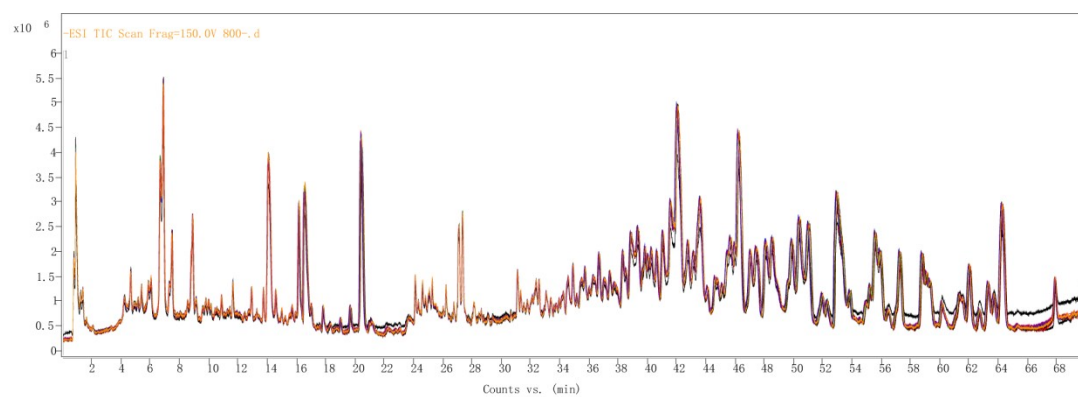
41 600 m



42

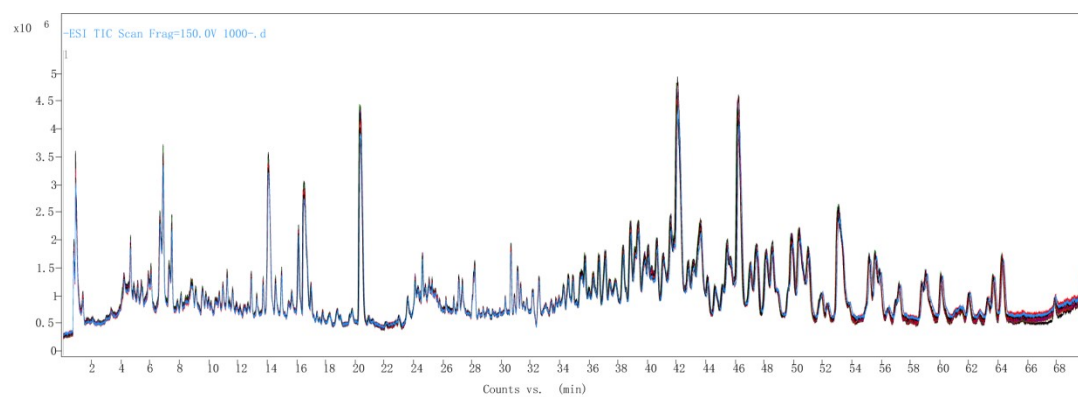
43

44 **800 m**



45

46 **1000 m**

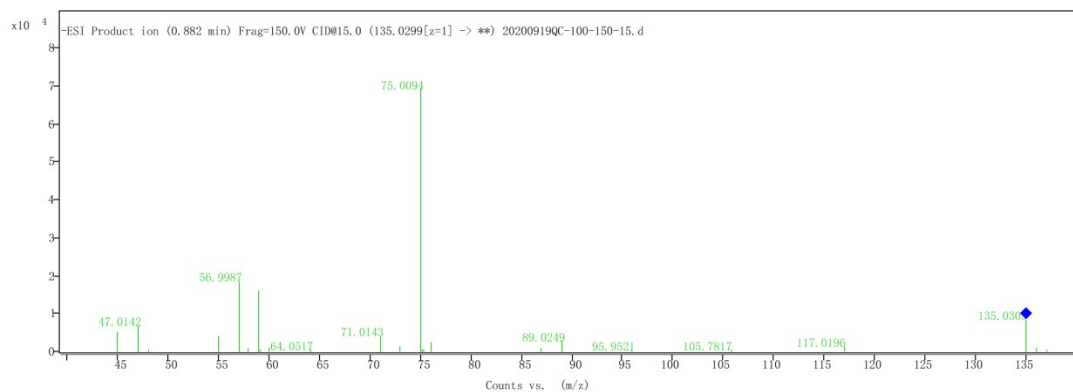


47

48

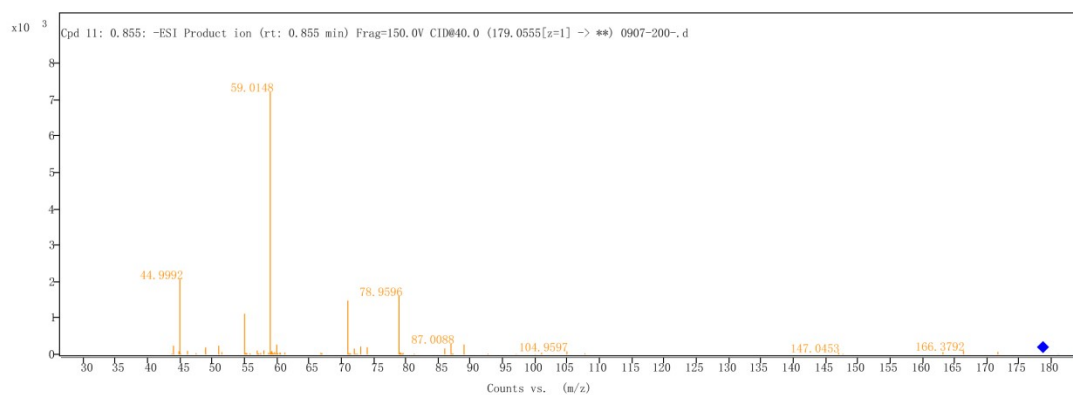
49 ● The MS/MS information of all identified compounds (Fig. S3)

50 1. Compound: Threonic acid M/Z 135.0299 Formula C₄H₈O₅



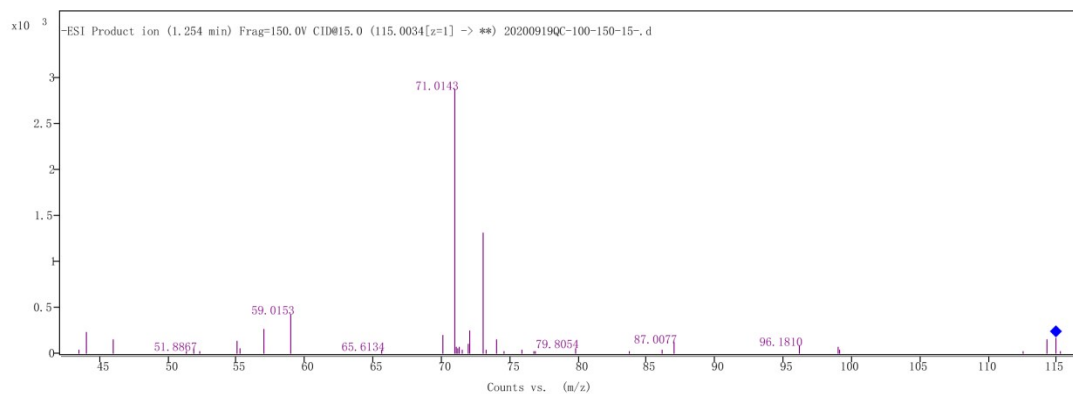
51

52 2. Compound: D-Fructose M/Z 179.0555 Formula C₆H₁₂O₆



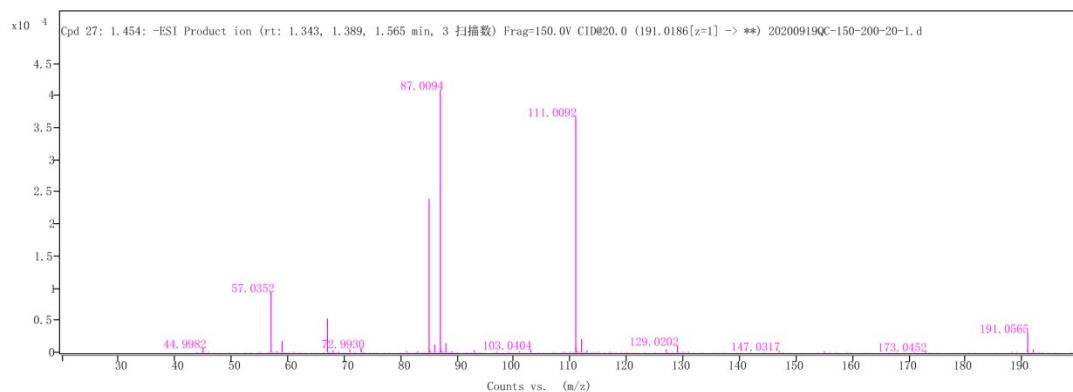
53

54 3. Compound: Fumaric acid M/Z 115.0034 Formula C₄H₄O₄



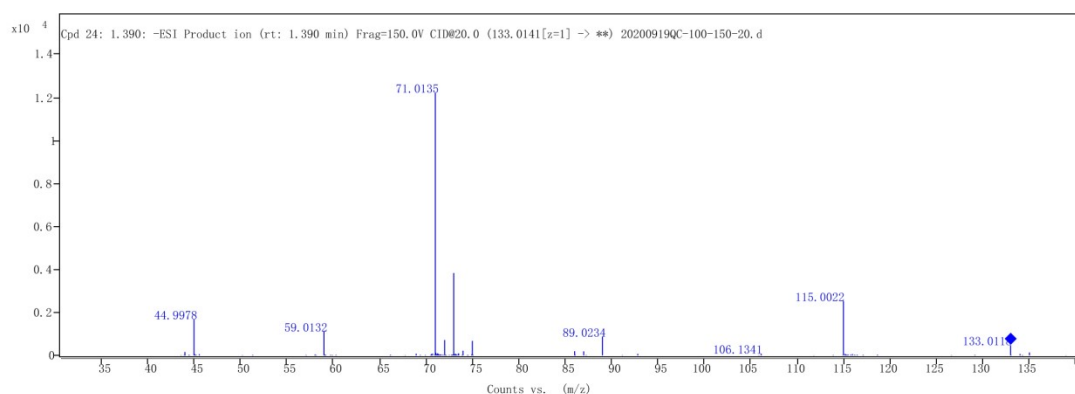
55

56 4. Compound: Quinic acid M/Z 191.0565 Formula C₇H₁₂O₆



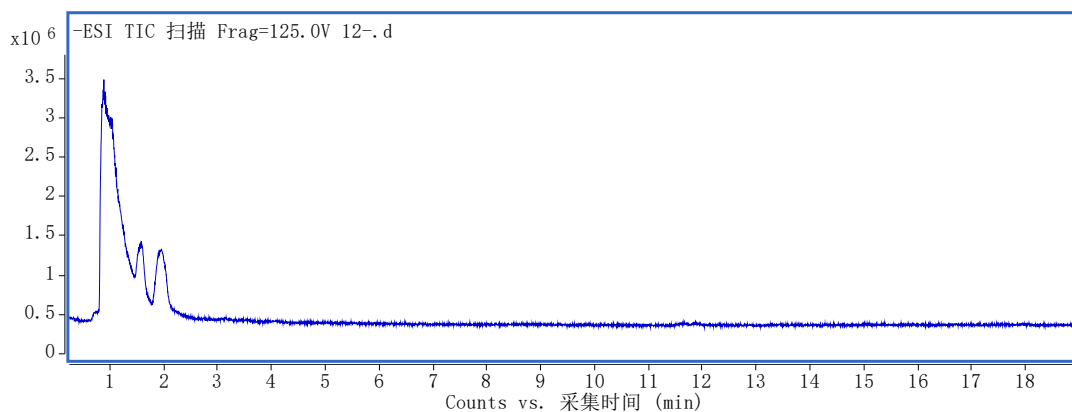
57

58 5. Compound: Malic acid M/Z 133.0141 Formula C₄H₆O₅



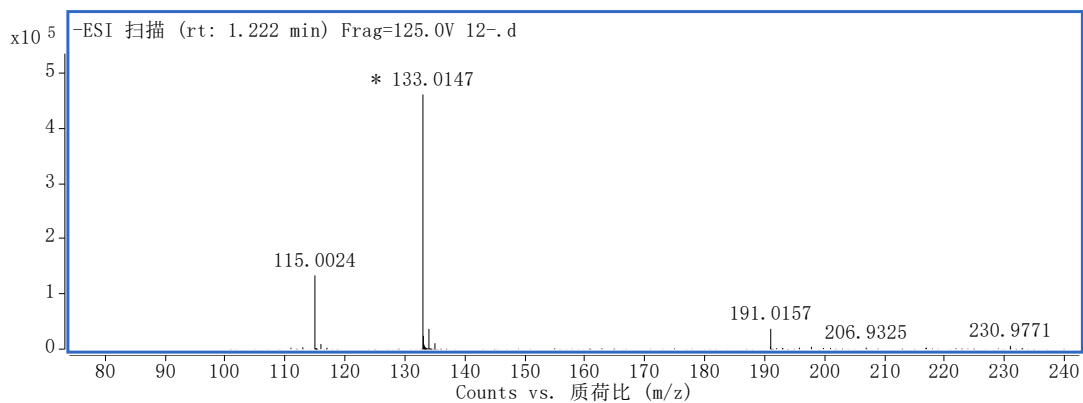
59

60 TIC of the standard



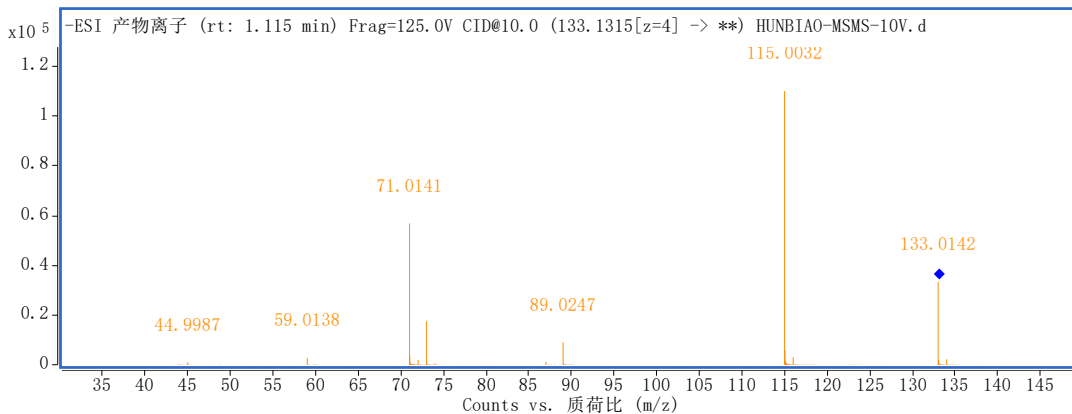
61

62 MS of the standard



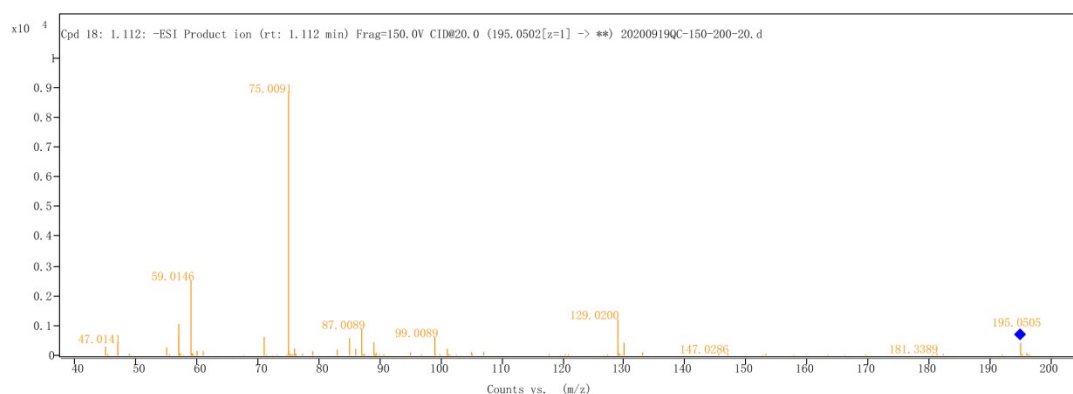
63

64 MS/MS of the standard



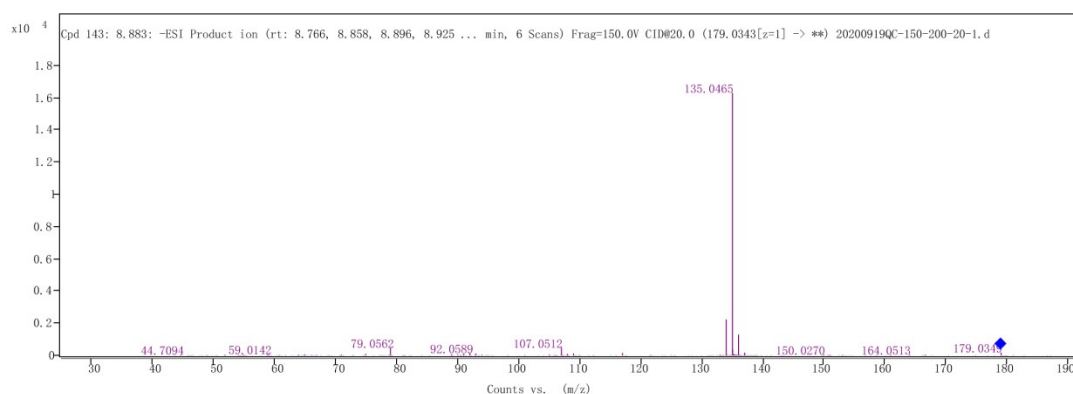
65

66 6. Compound: Gluconic acid M/Z 195.0505 Formula C₆H₁₂O₇



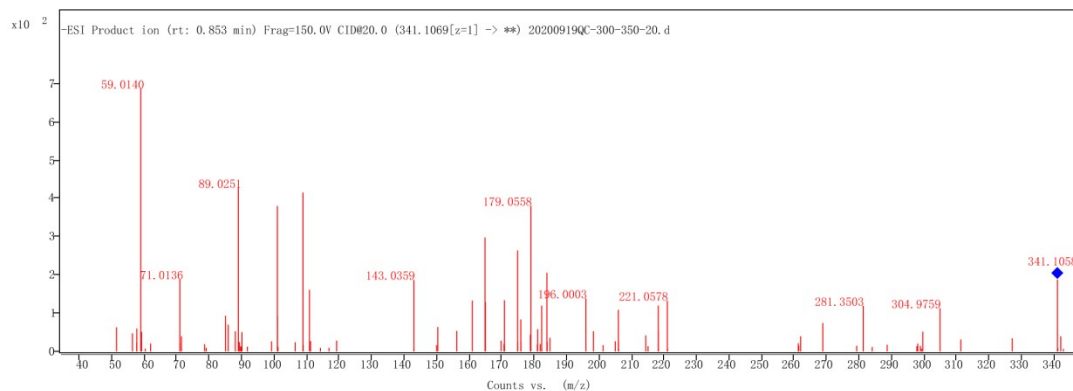
67

68 7. Compound: D-Galactose M/Z 179.0562 Formula C₆H₁₂O₆



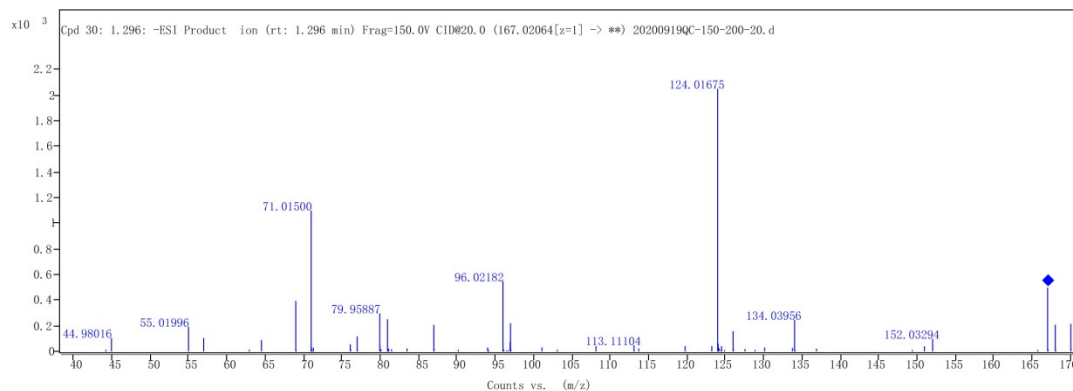
69

70 8. Compound: Sucrose M/Z 341.1090 Formula C₁₂H₂₂O₁₁



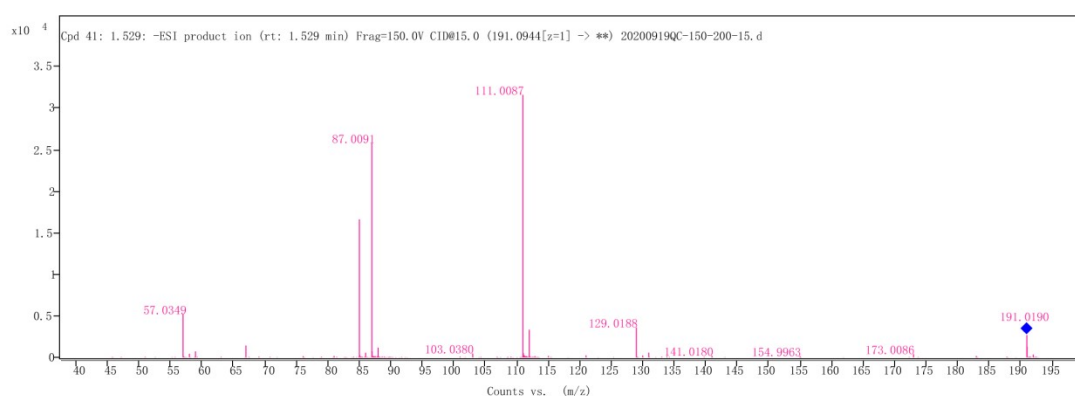
71

72 9. Compound: Uric acid M/Z 167.0206 Formula C₅H₄N₄O₃



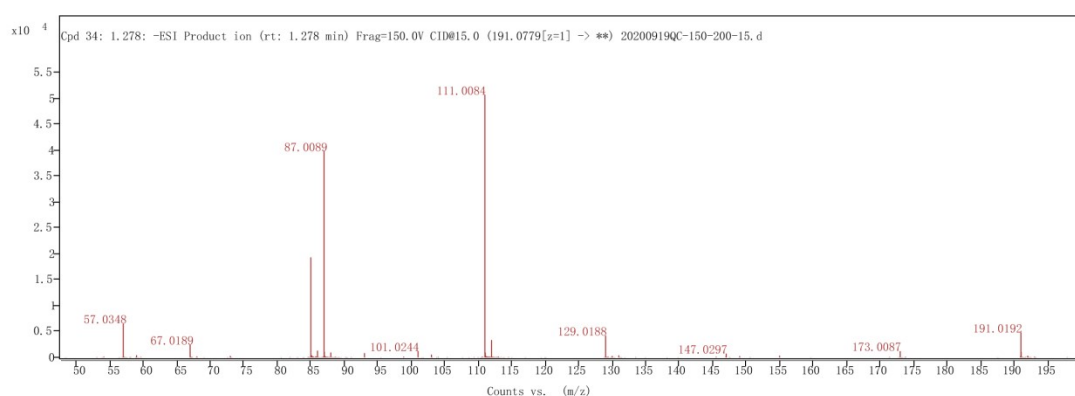
73

74 10. Compound: Isocitric acid M/Z 191.0190 Formula C₆H₈O₇



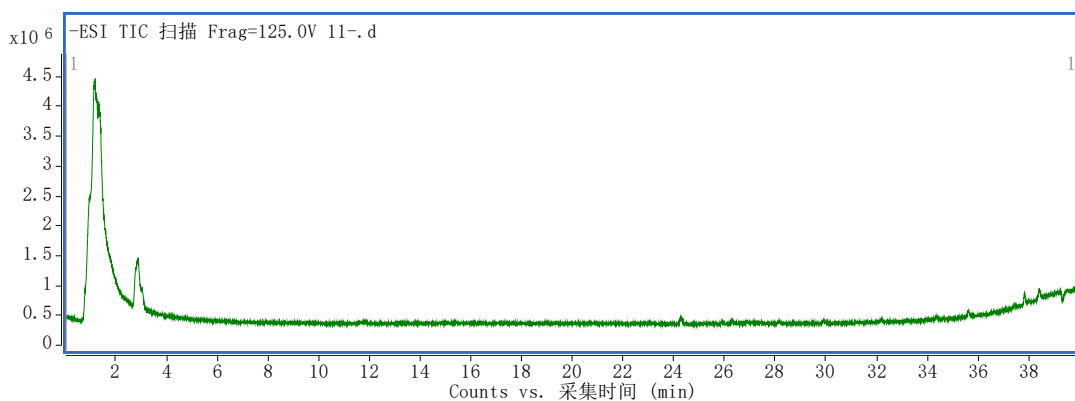
75

76 11. Compound: Citric acid M/Z 191.0192 Formula C₆H₈O₇



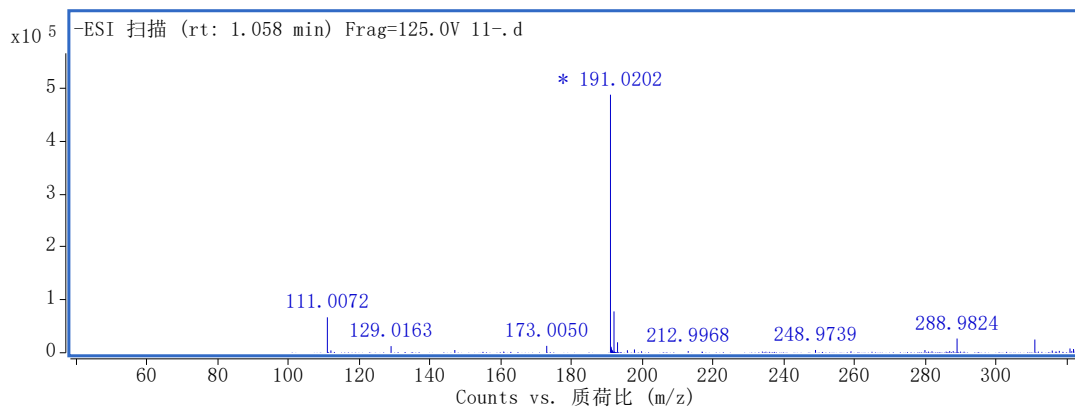
77

78 TIC of the standard



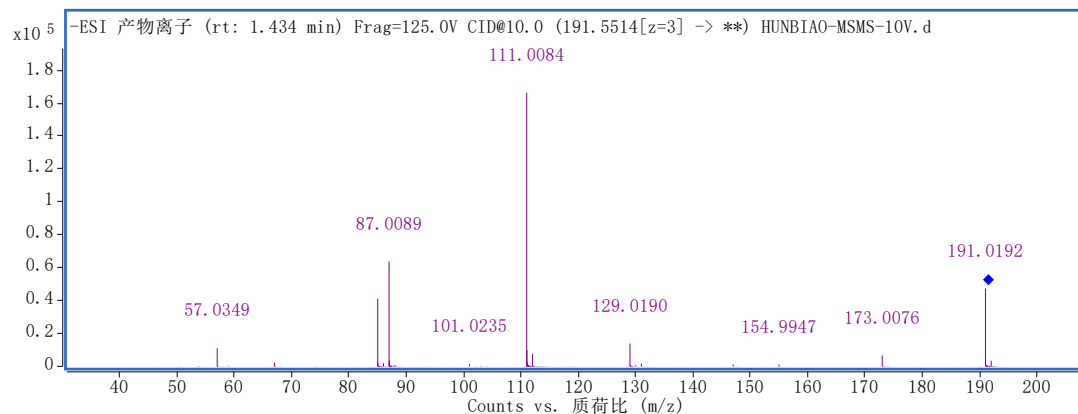
79

80 MS of the standard



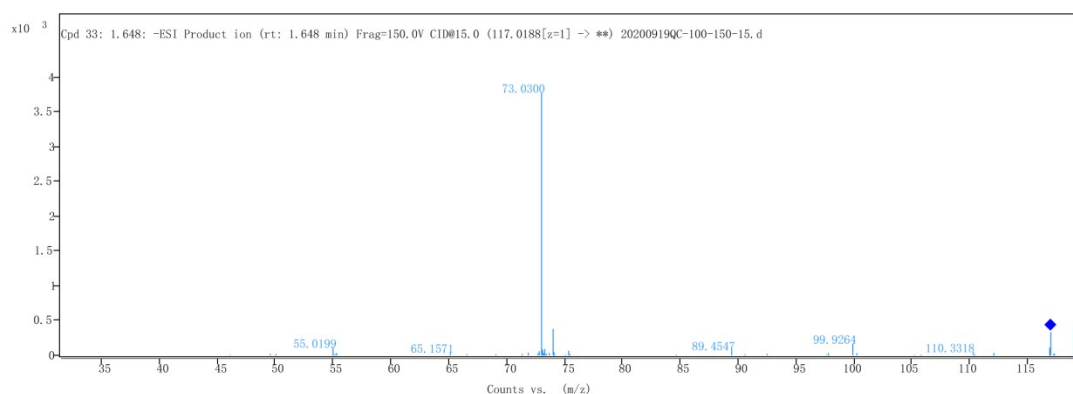
81

82 MS/MS of the standard



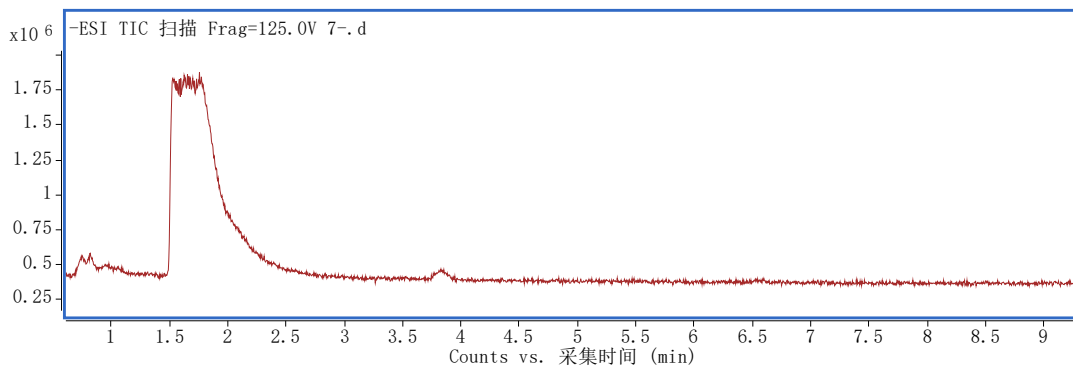
83

84 12. Compound: Succinic acid M/Z 117.0188 Formula C₄H₆O₄



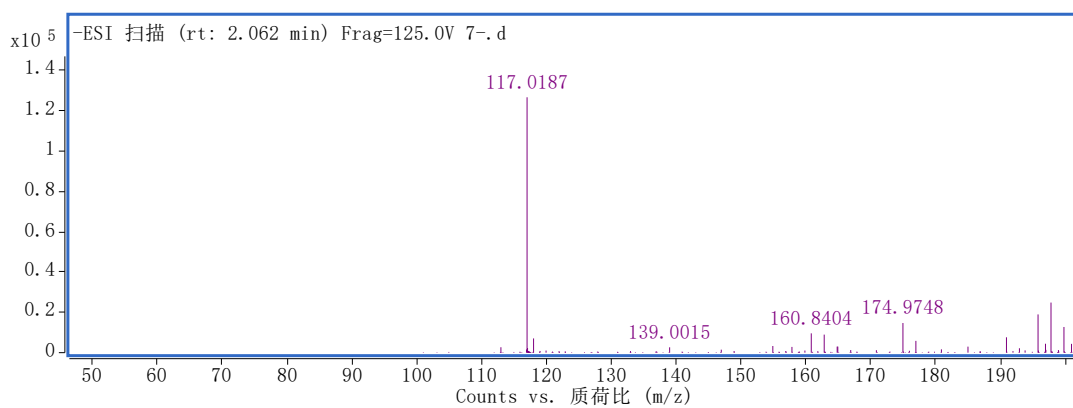
85

86 TIC of the standard



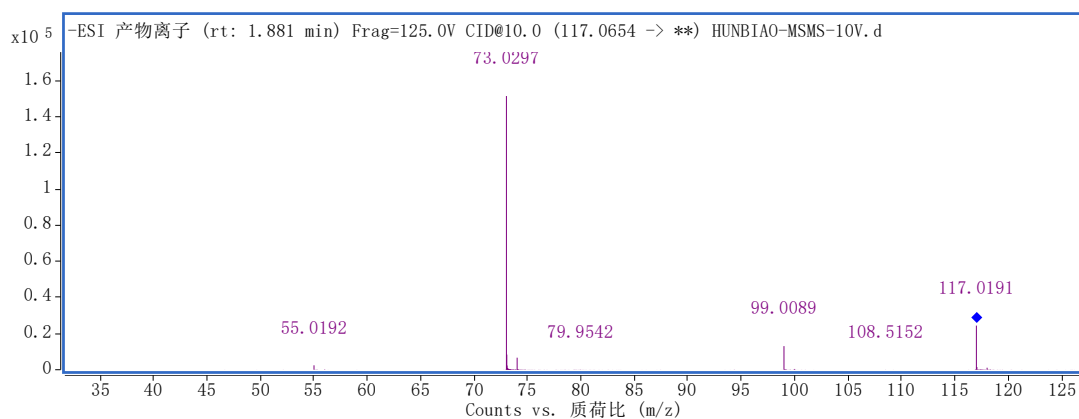
87

88 MS of the standard

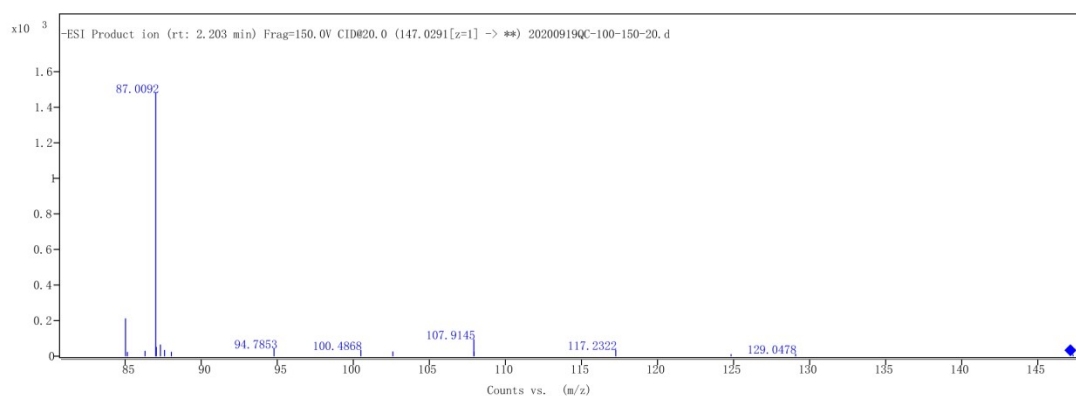


89

90 MS/MS of the standard

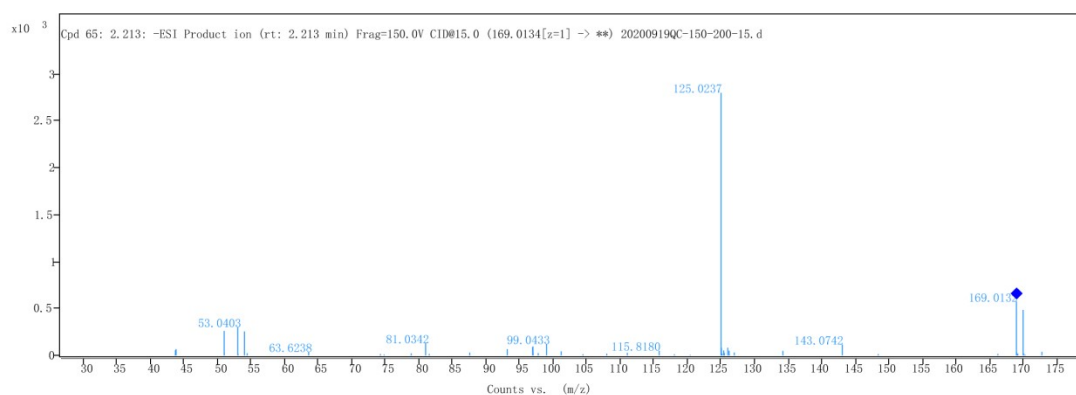


92 13. Compound: Citramalic acid M/Z 147.0297 Formula C₅H₈O₅



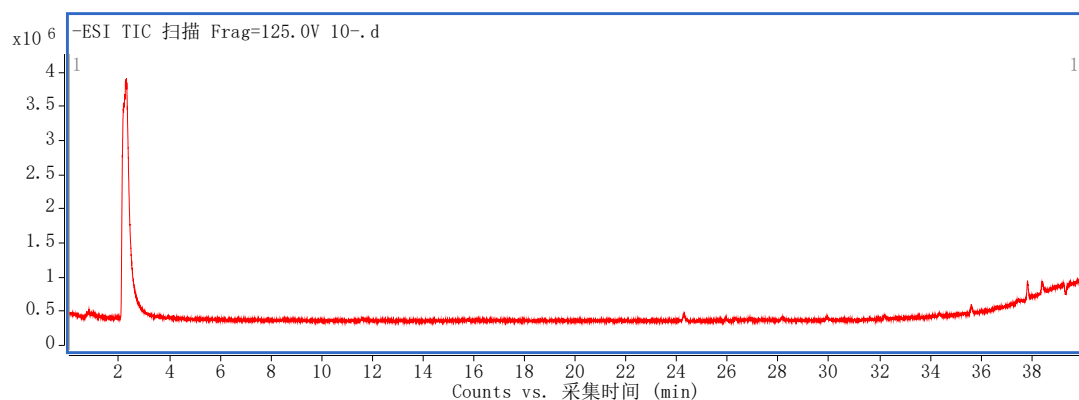
93

94 14. Compound: Gallic acid M/Z 169.0134 Formula C₇H₆O₅



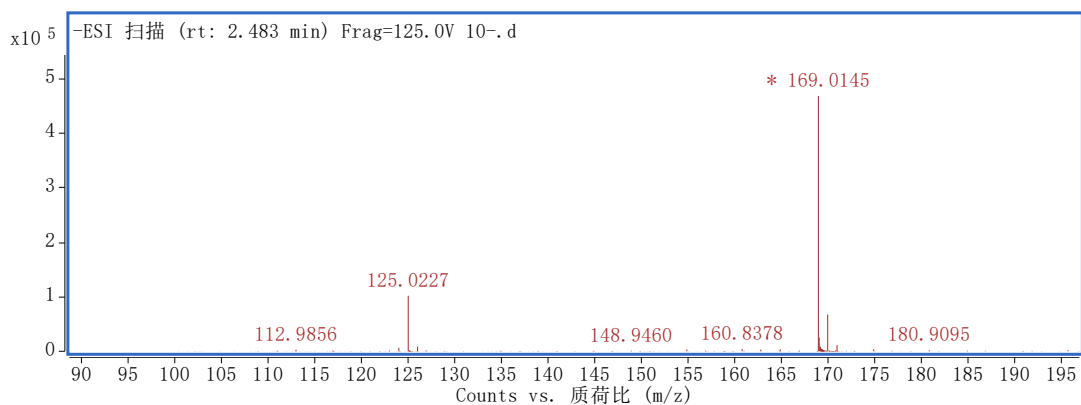
95

96 TIC of the standard

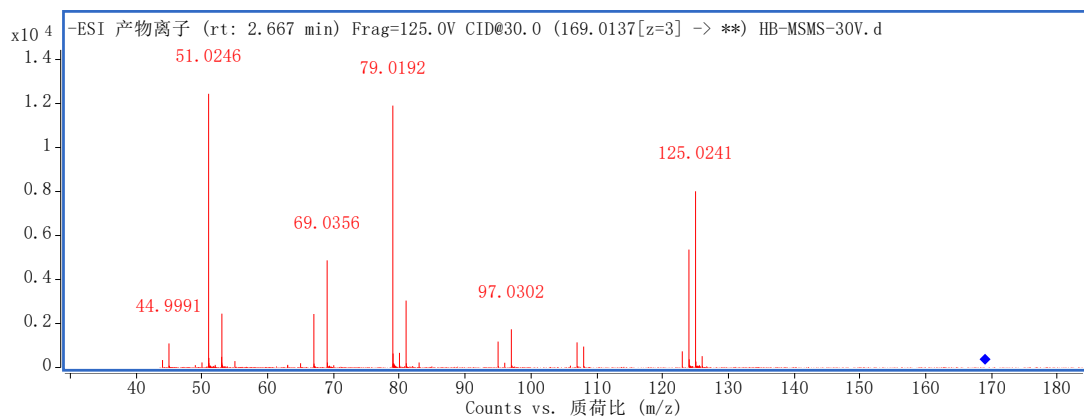


97

98 MS of the standard

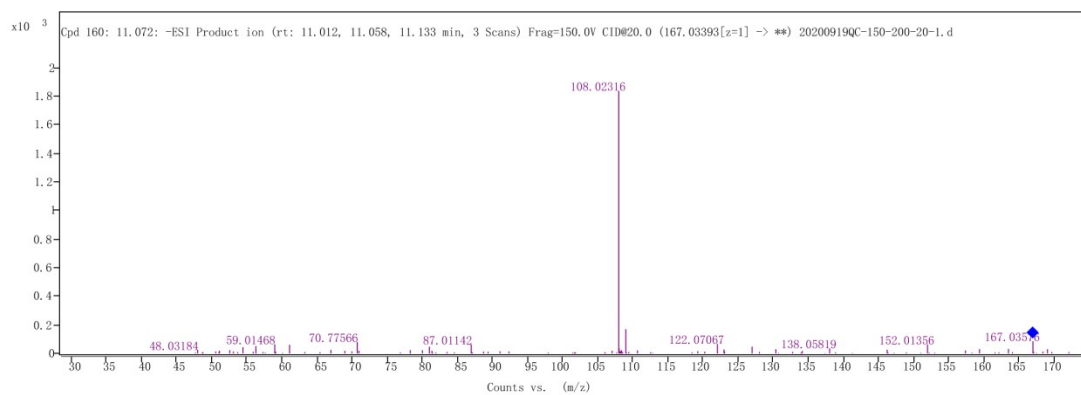


100 MS/MS of the standard



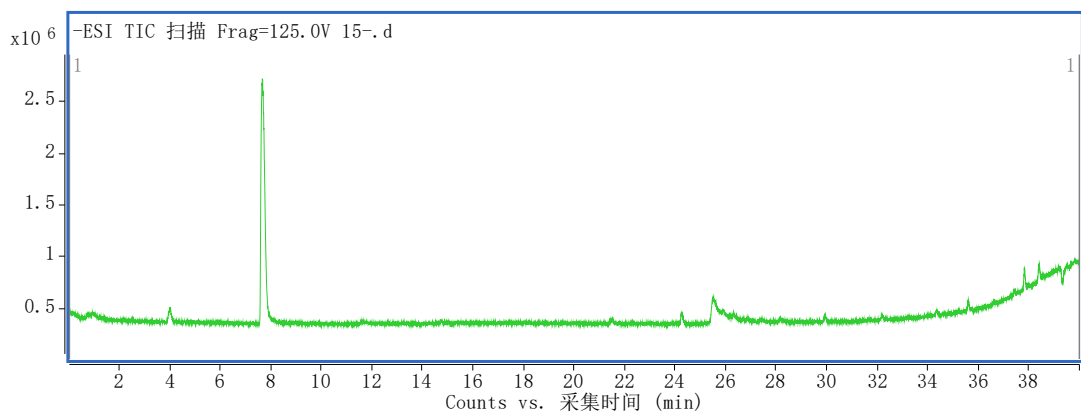
101

102 15. Compound: Vanillic acid M/Z 167.0358 Formula C₈H₈O₄



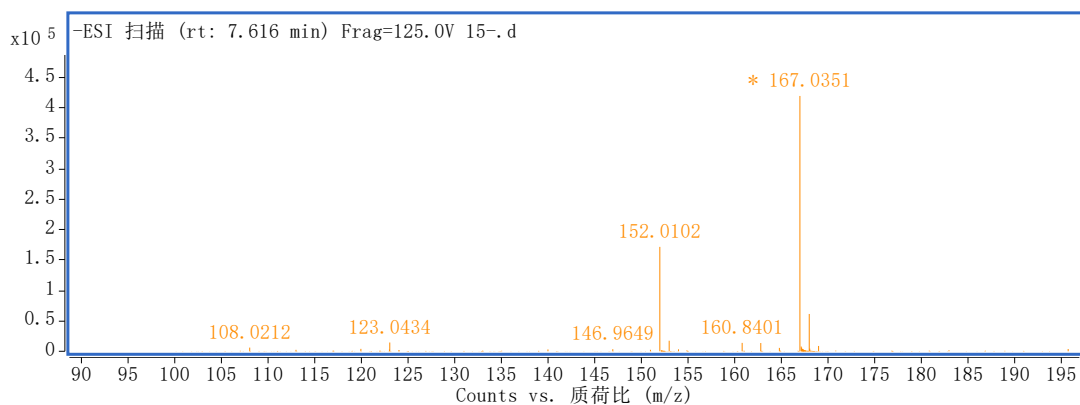
103

104 TIC of the standard

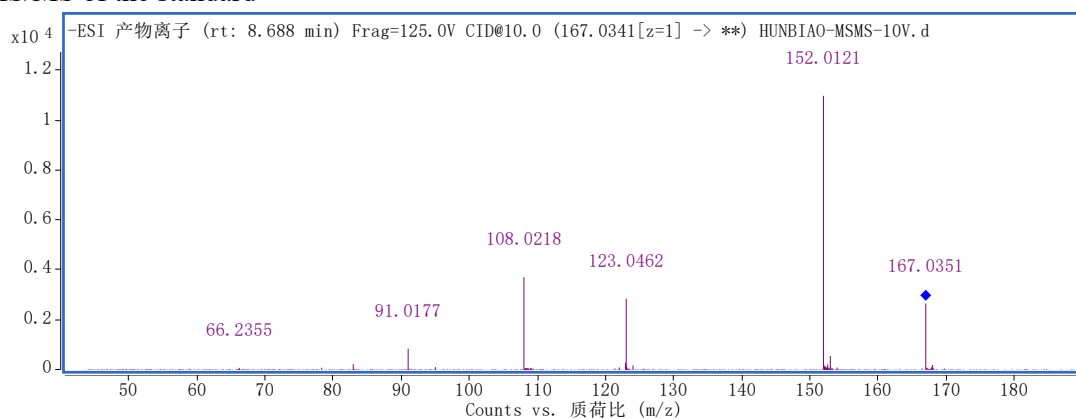


105

106 MS of the standard

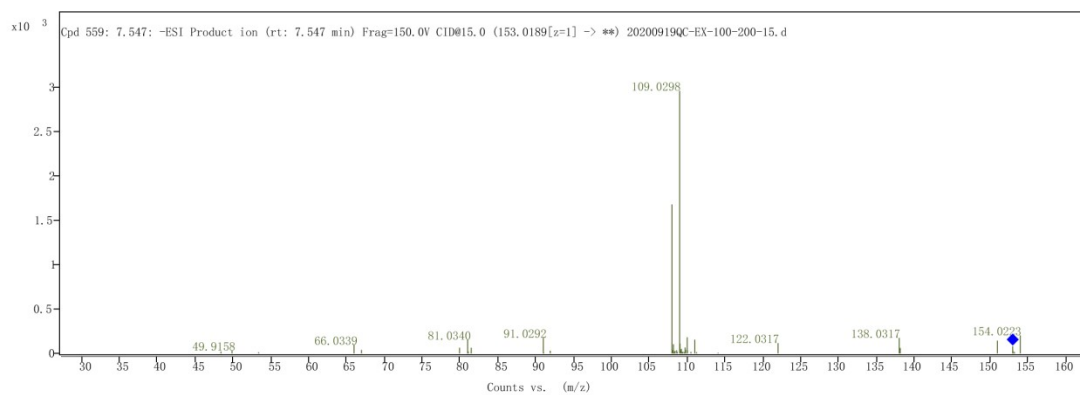


108 MS/MS of the standard



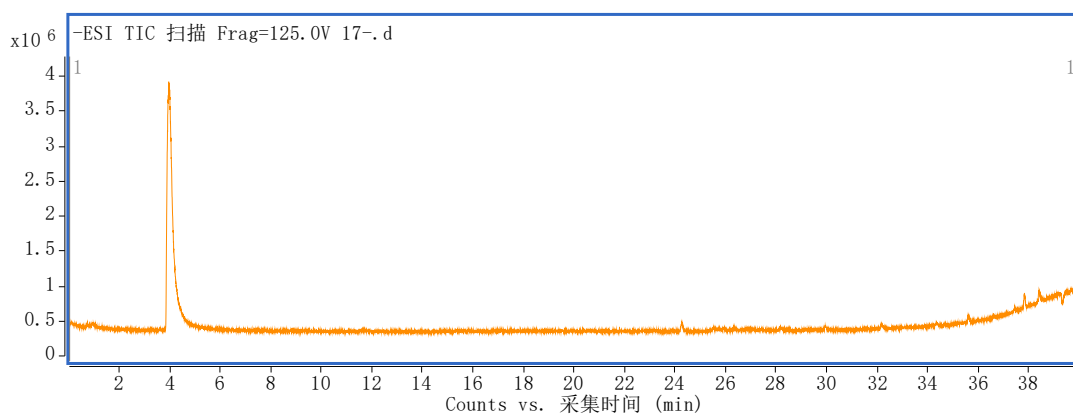
109

110 16. Compound: Protocatechuic acid M/Z 153.0189 Formula C₇H₆O₄



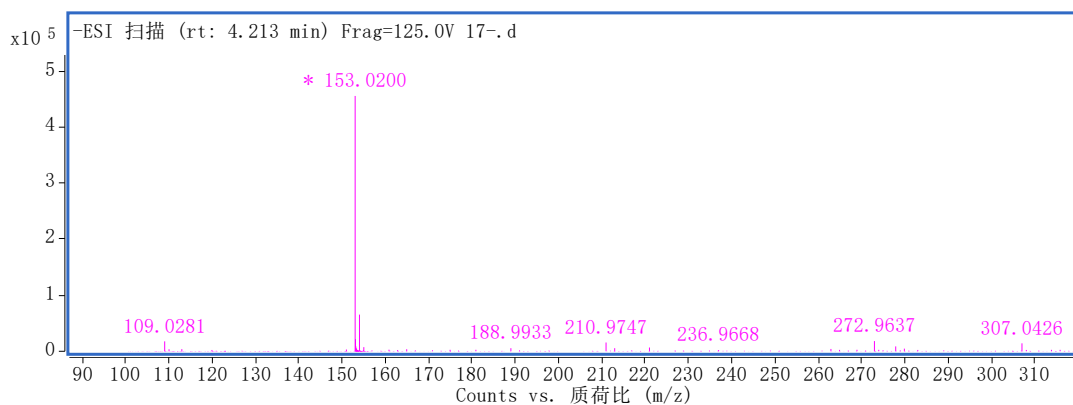
111

112 TIC of the standard

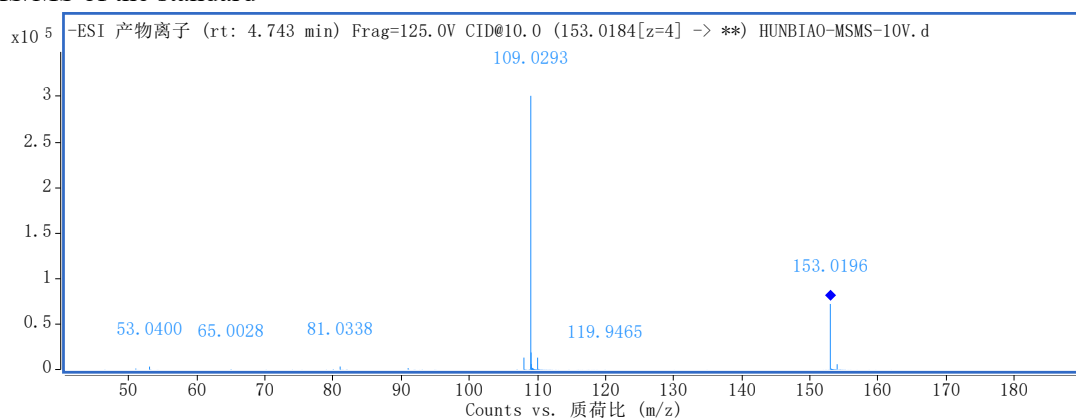


113

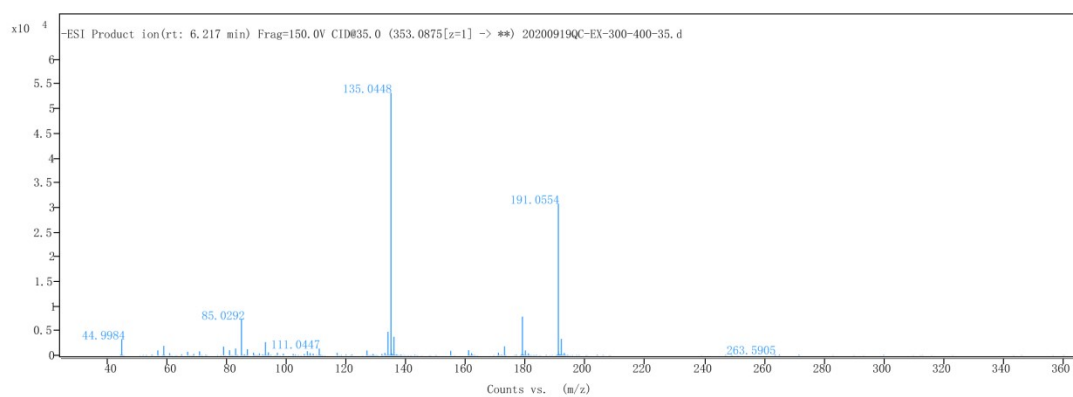
114 MS of the standard



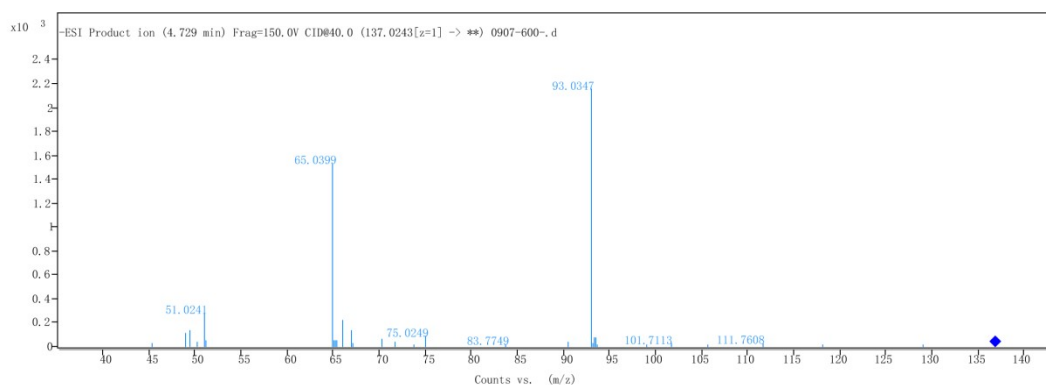
116 MS/MS of the standard



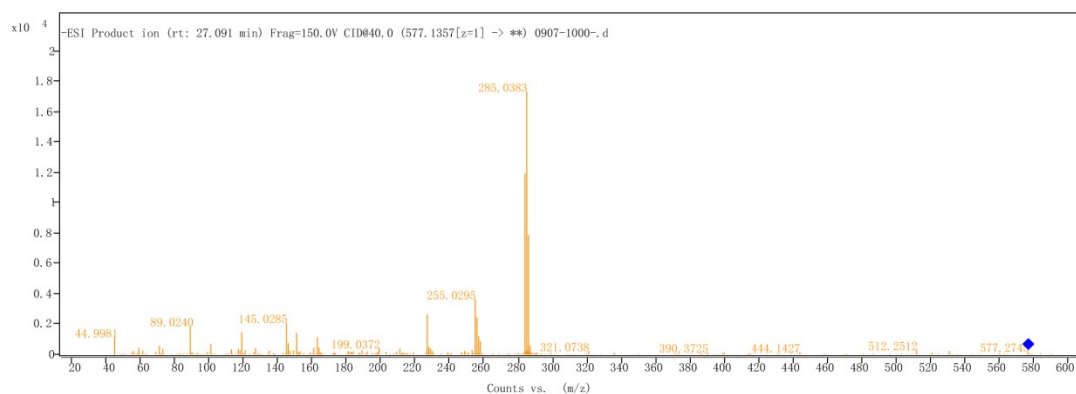
117 17. Compound: 4-Caffeoylquinic acid M/Z 353.0875 Formula C₁₆H₁₈O₉



119 18. Compound: Salicylic acid M/Z 137.0242 Formula C₇H₆O₃

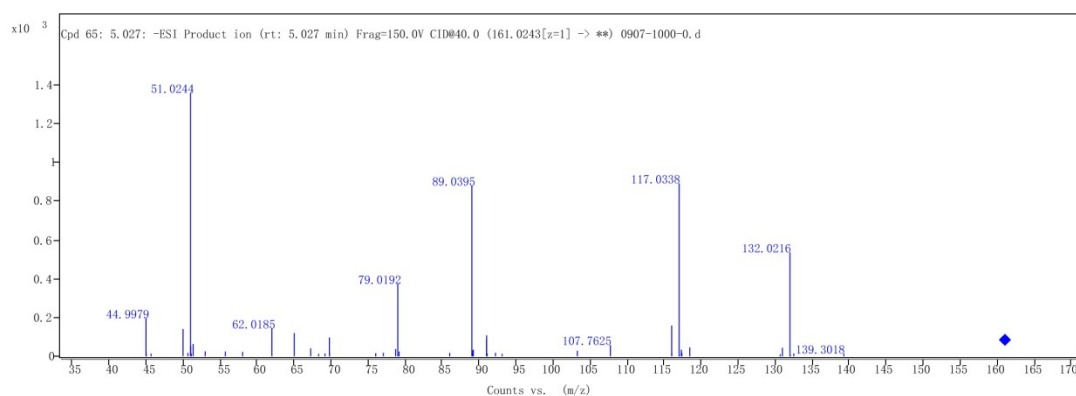


121 19. Compound: Procyanidin B1 M/Z 577.1331 Formula C₃₀H₂₆O₁₂



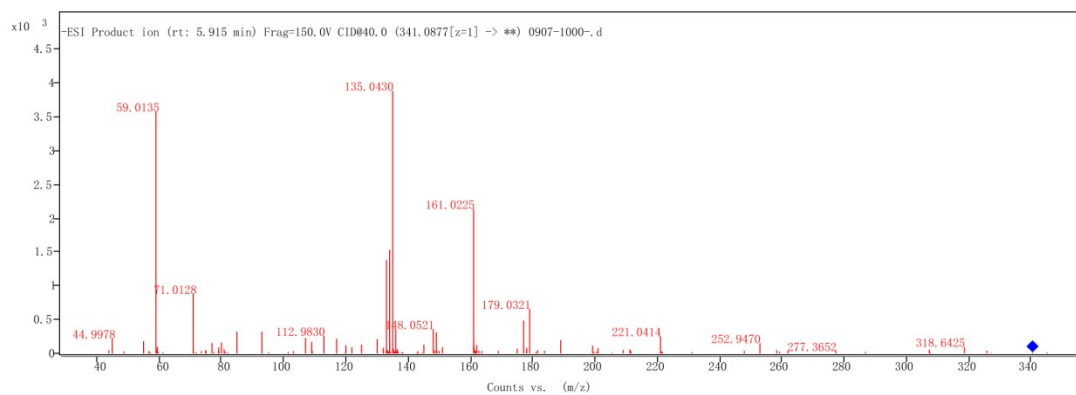
123

124 20. Compound: 4-Hydroxycoumarin M/Z 161.0243 Formula C₉H₆O₃



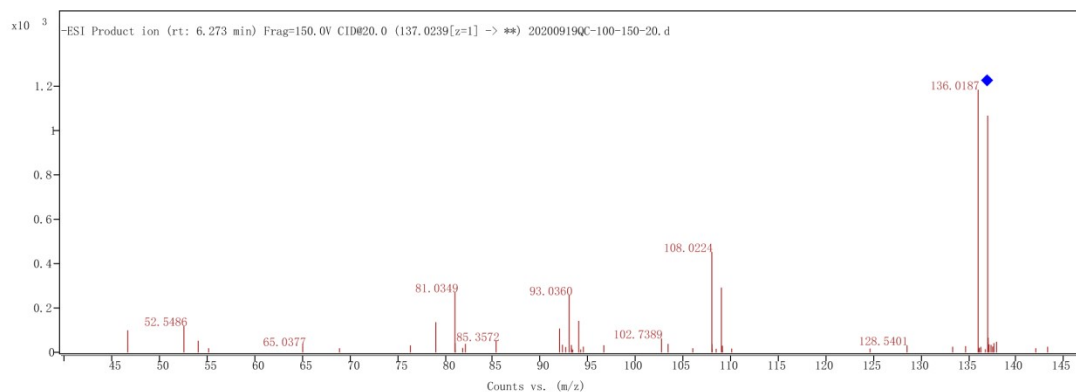
125

126 21. Compound: Glucocaffeic acid M/Z 341.0877 Formula C₁₅H₁₈O₉



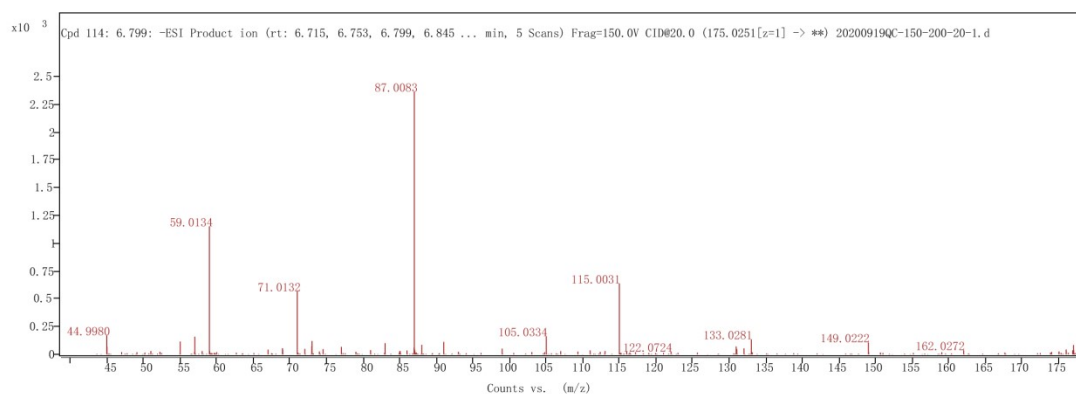
127

128 22. Compound: 3,4-Dihydroxybenzaldehyde M/Z 137.0245 Formula C₇H₆O₃



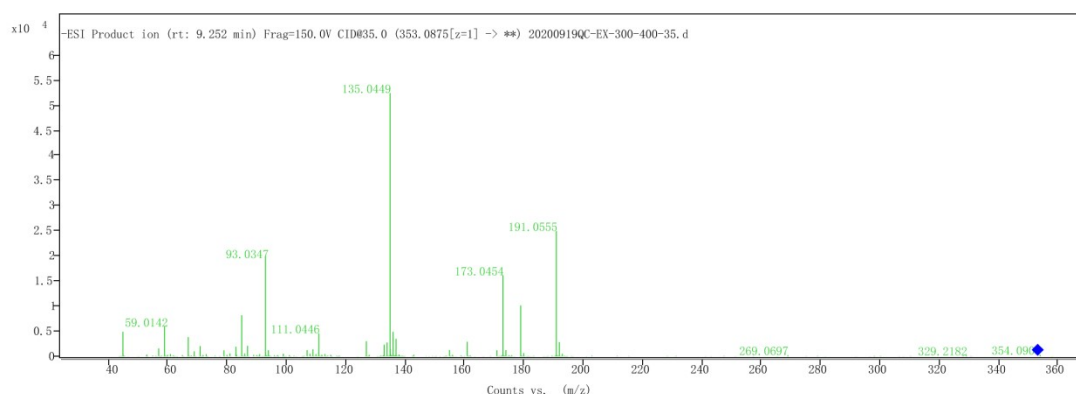
129

130 23. Compound: L-Ascorbic acid M/Z 175.0251 Formula C₆H₈O₆



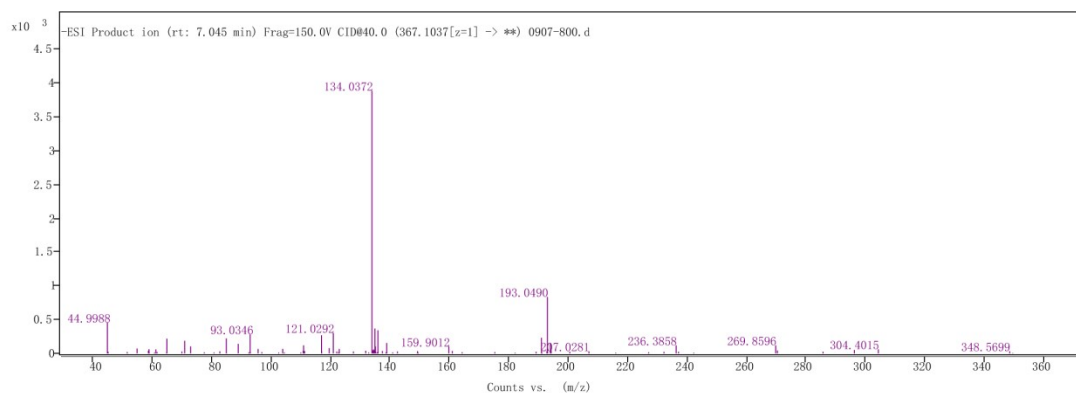
131

132 24. Compound: Chlorogenic acid M/Z 353.0890 Formula C₁₆H₁₈O₉



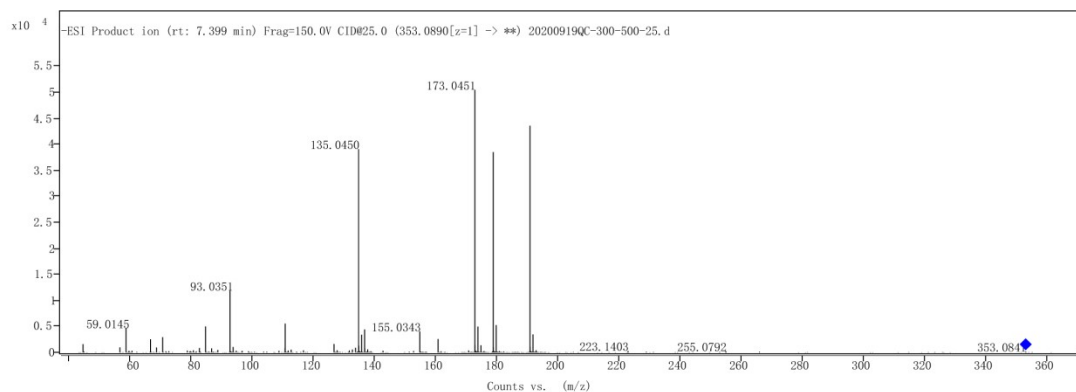
133

134 25. Compound: 3-Feruloylquinic acid M/Z 367.1037 Formula C₁₇H₂₀O₉



135

136 26. Compound: 1-Caffeoylquinic acid M/Z 353.0890 Formula C₁₆H₁₈O₉

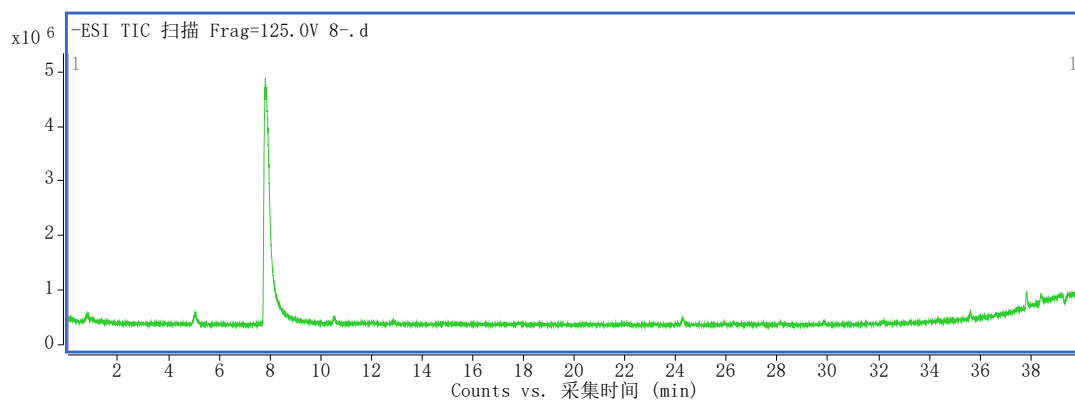


137

138 27. Compound: Caffeic acid M/Z 179.0349 Formula C₉H₈O₄

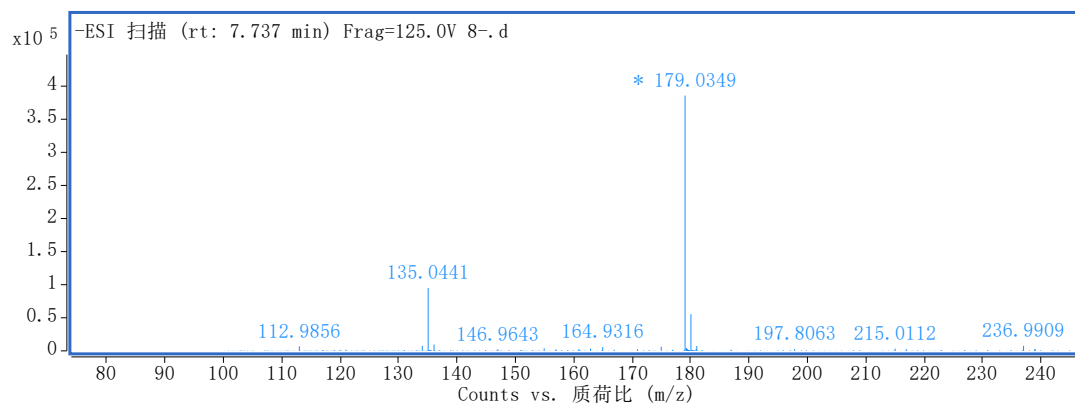
139

140 TIC of the standard



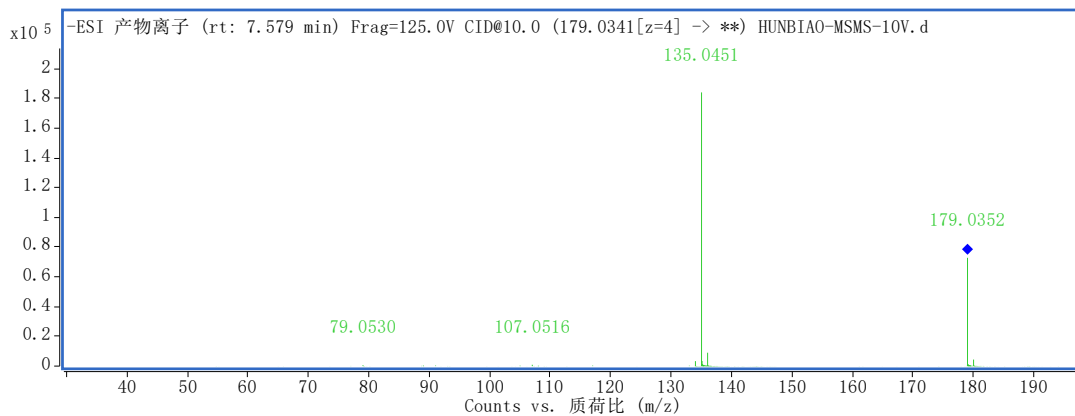
141

142 MS of the standard



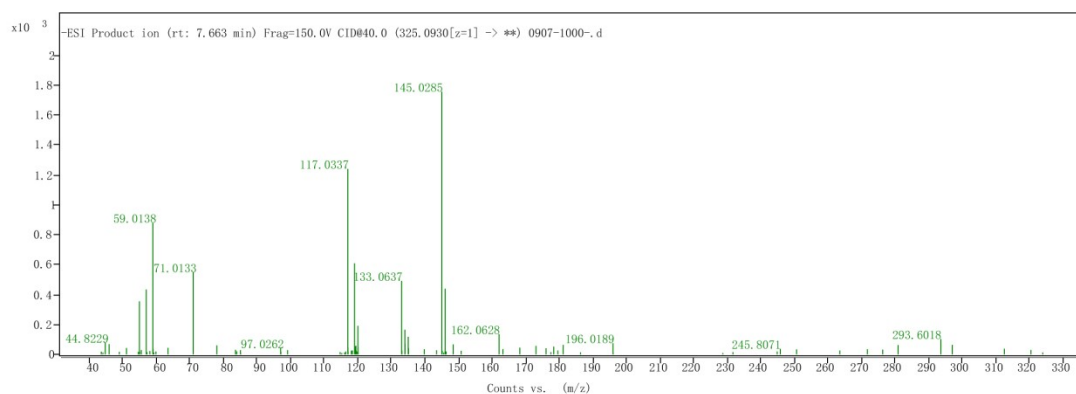
143

144 MS/MS of the standard



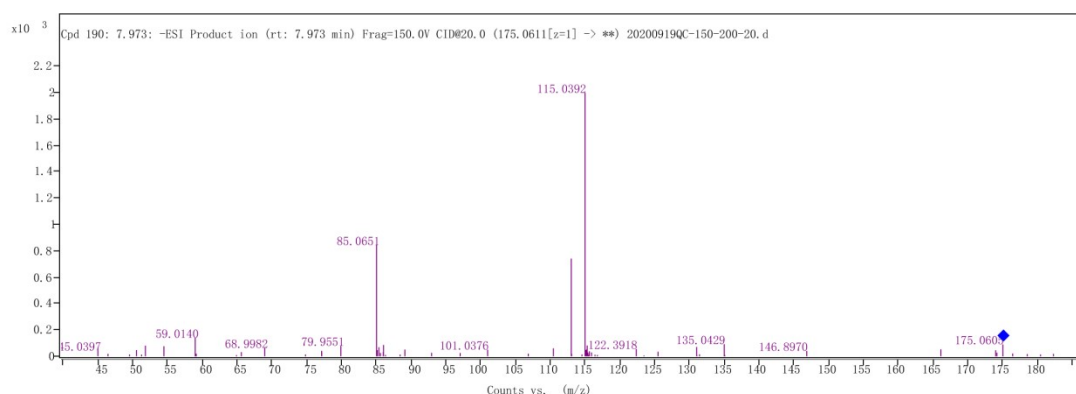
145

146 28. Compound: Bilobalide M/Z 325.0930 Formula C₁₅H₁₈O₈



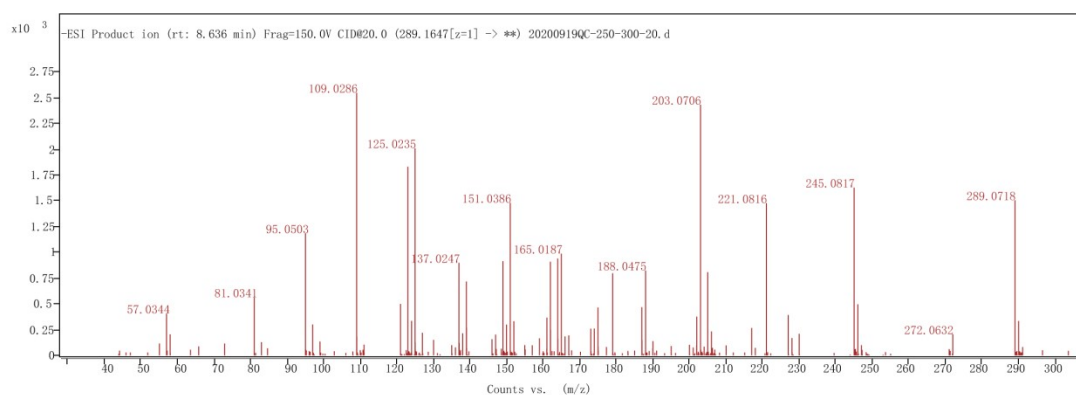
147

148 29. Compound: 2-Isopropylmalic acid M/Z 175.0605 Formula C7H12O5



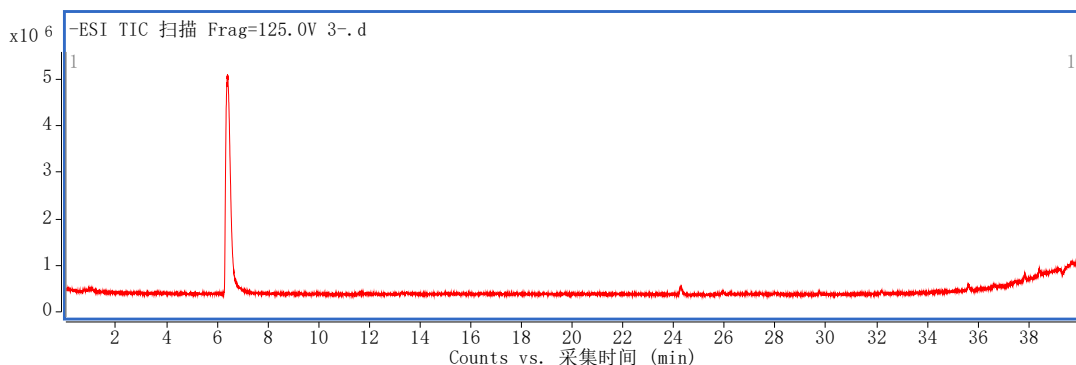
149

150 30. Compound: Catechin M/Z 289.0718 Formula C15H14O6



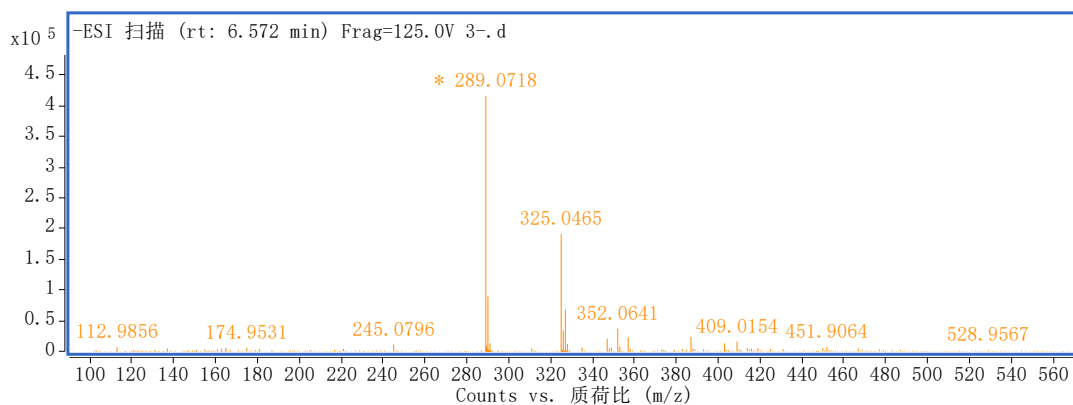
151

152 TIC of the standard



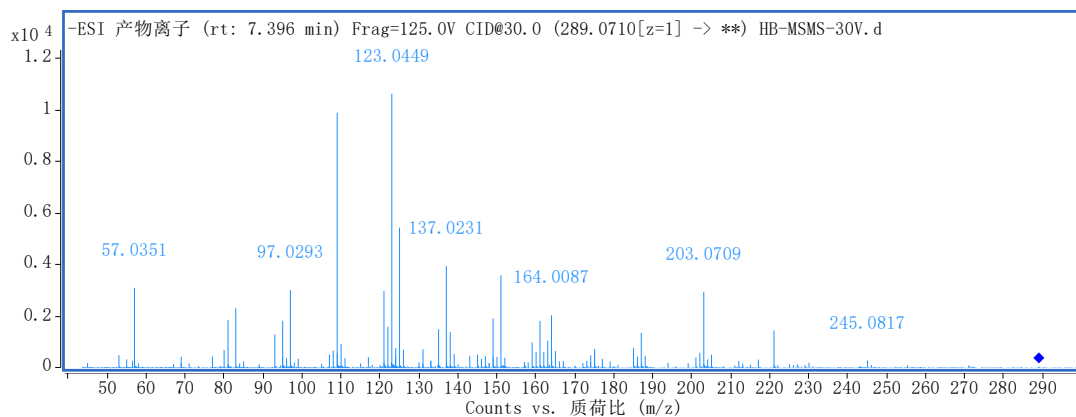
153

154 MS of the standard



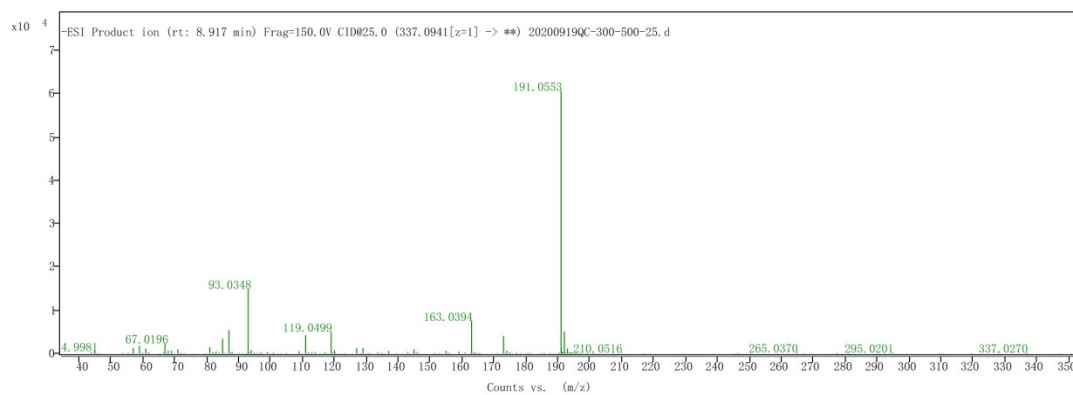
155

156 MS/MS of the standard



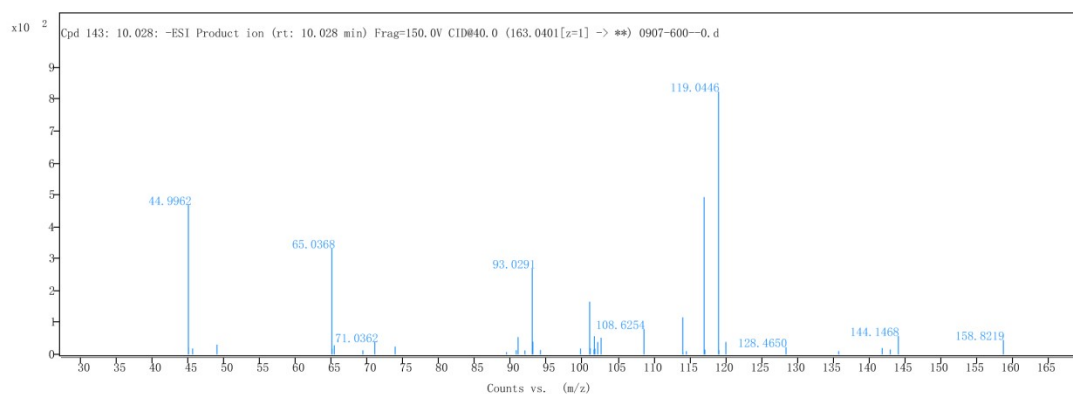
157

158 31. Compound: 3-O-p-Coumaroylquinic acid M/Z 337.0941 Formula C₁₆H₁₈O₈



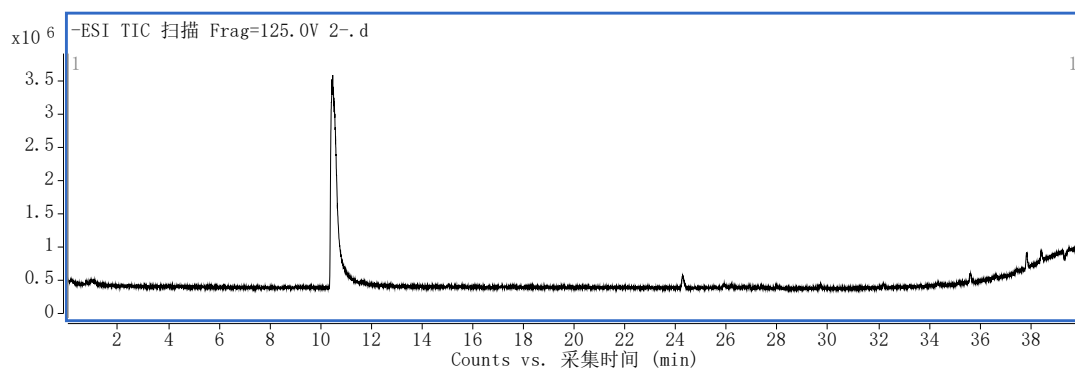
159

160 32. Compound: p-Coumaric acid M/Z 163.0401 Formula C₉H₈O₃



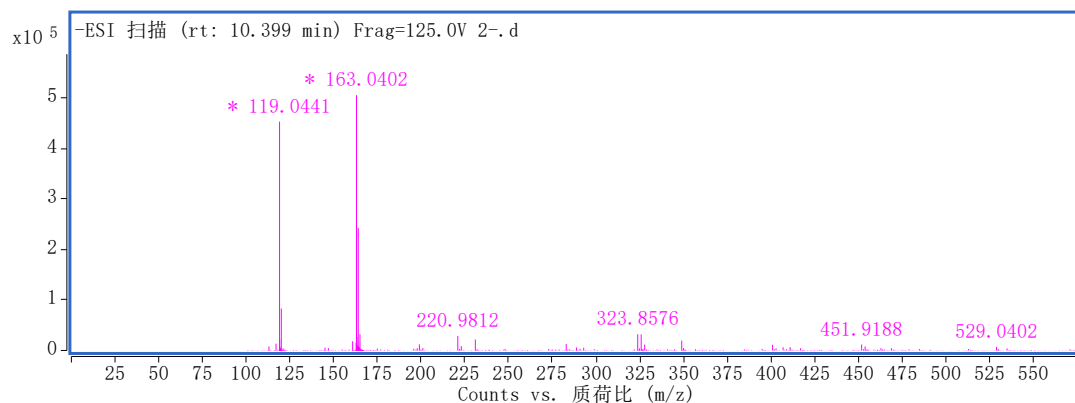
161

162 TIC of the standard



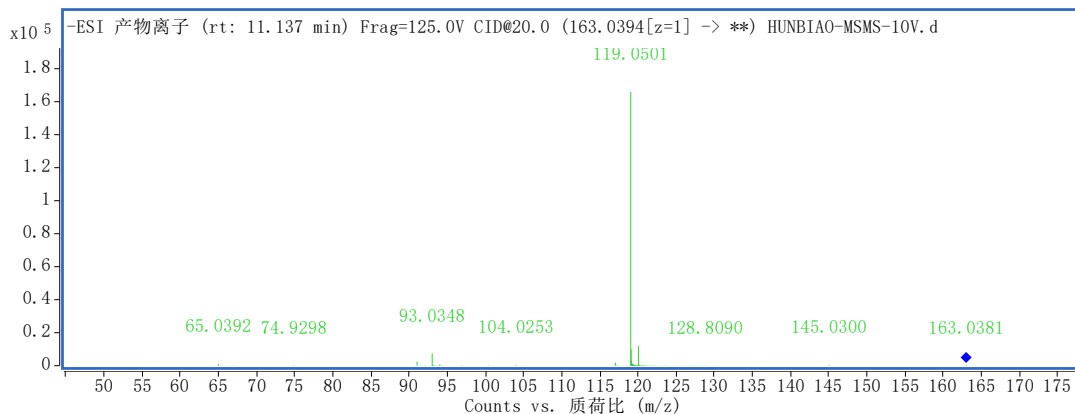
163

164 MS of the standard



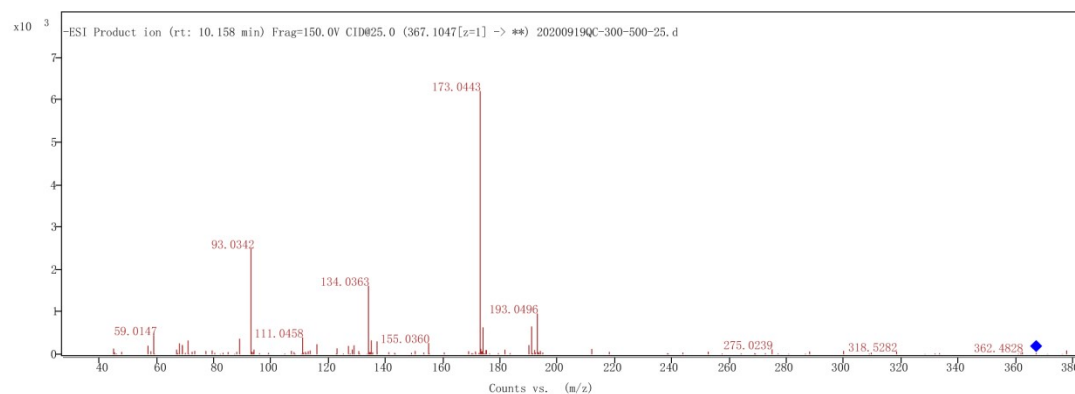
165

166 MS/MS of the standard



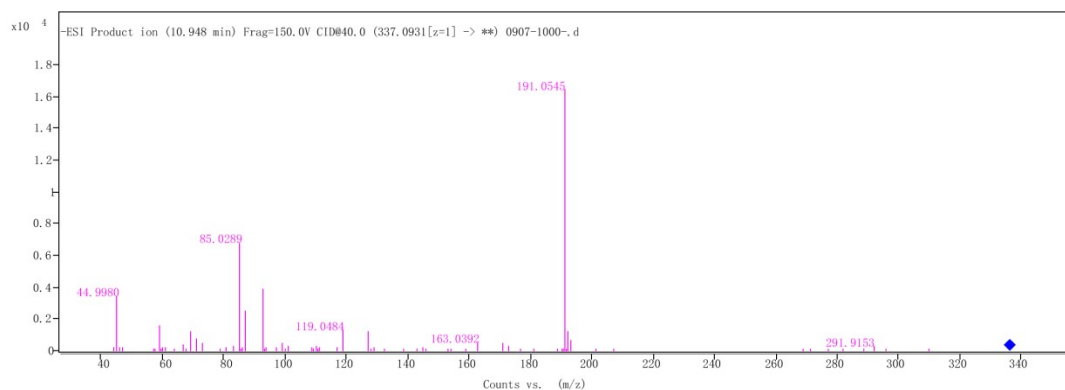
167

168 33. Compound: 4-Feruloylquinic acid M/Z 367.1047 Formula C₁₇H₂₀O₉



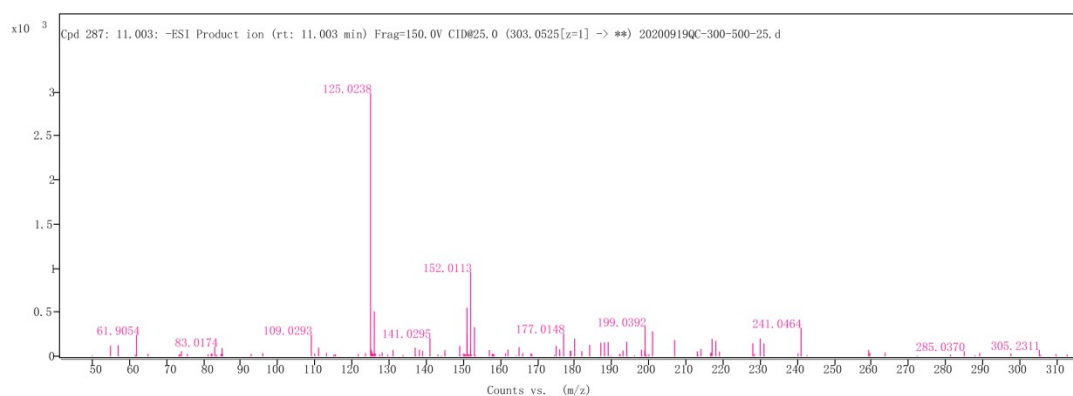
169

170 34. Compound: 5-p-Coumaroylquinic acid M/Z 337.0931 Formula C₁₆H₁₈O₈



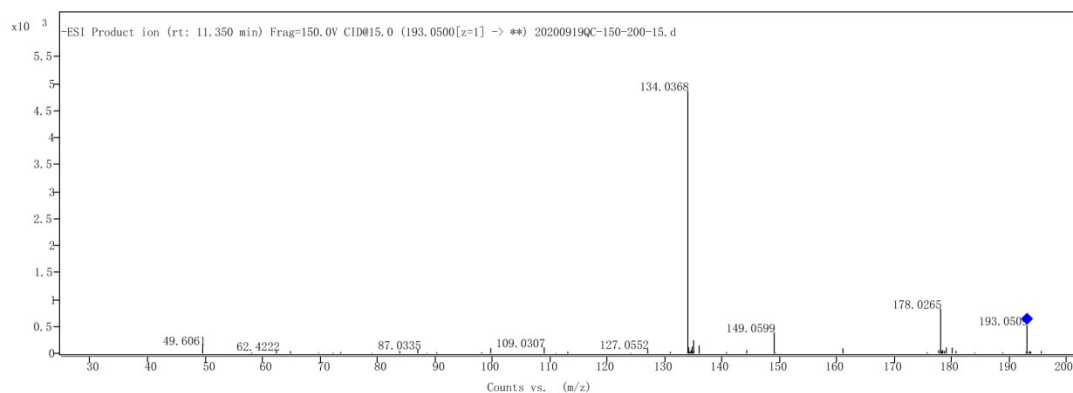
171

172 35. Compound: Taxifolin M/Z 303.0525 Formula C₁₅H₁₂O₇



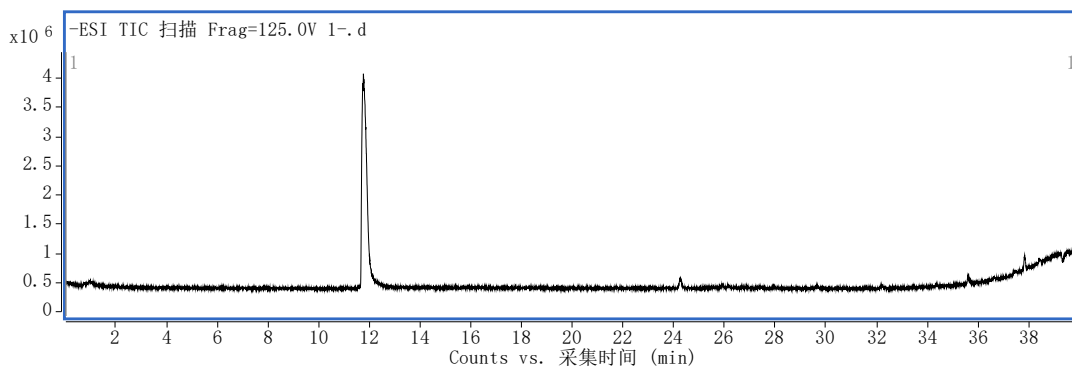
173

174 36. Compound: Ferulic acid M/Z 193.0509 Formula C₁₀H₁₀O₄



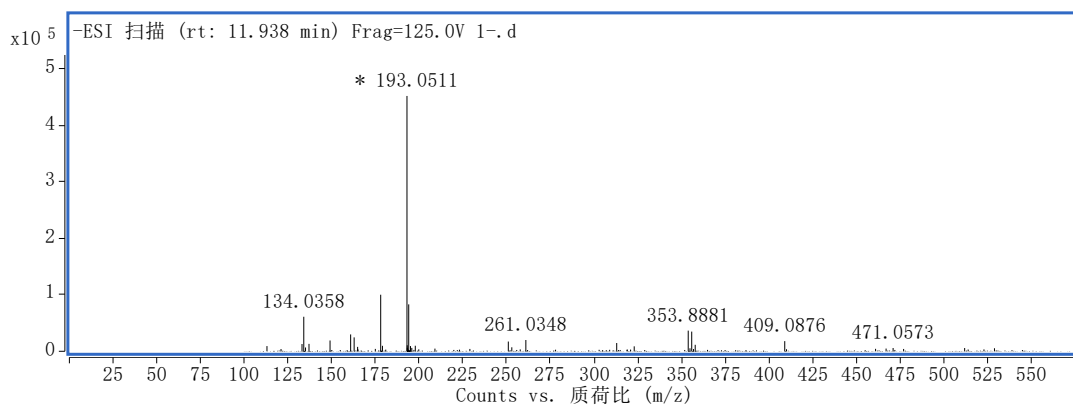
175

176 TIC of the standard

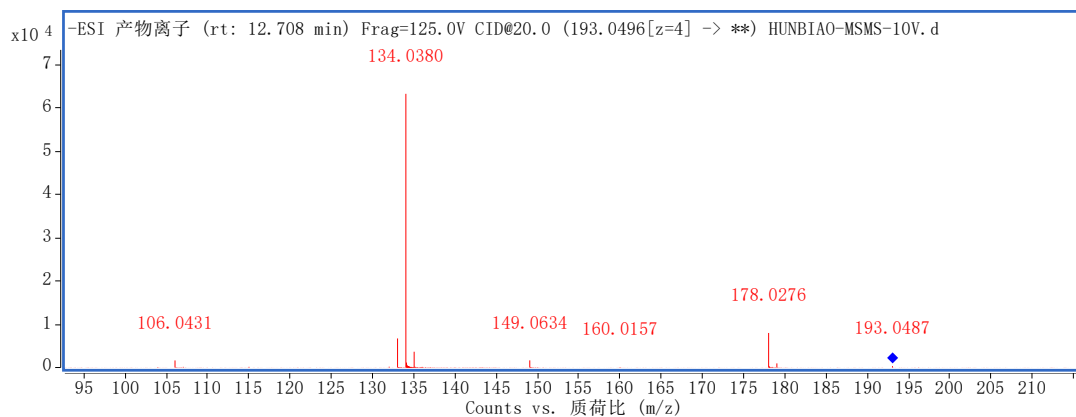


177

178 MS of the standard

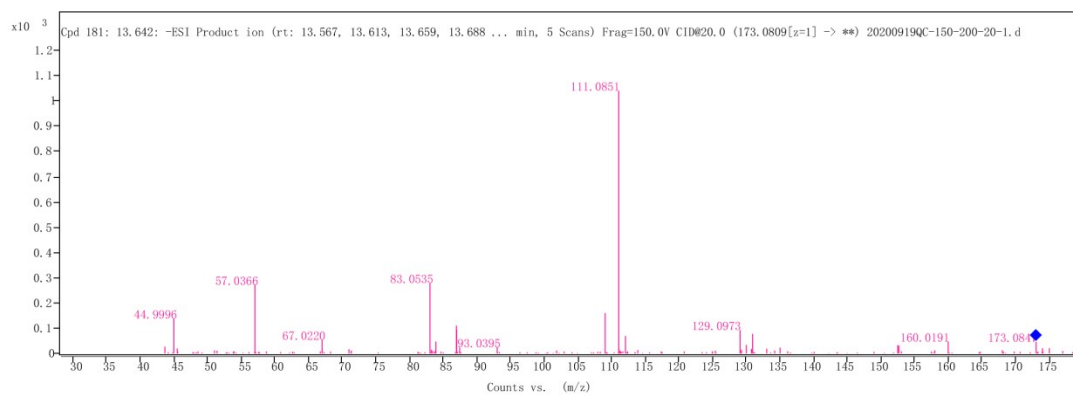


180 MS/MS of the standard



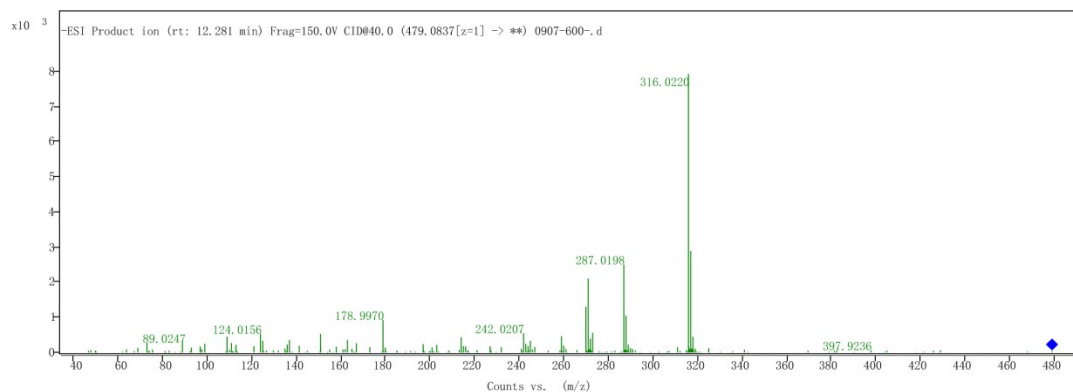
181

182 37. Compound: Suberic acid M/Z 173.0814 Formula C₈H₁₄O₄



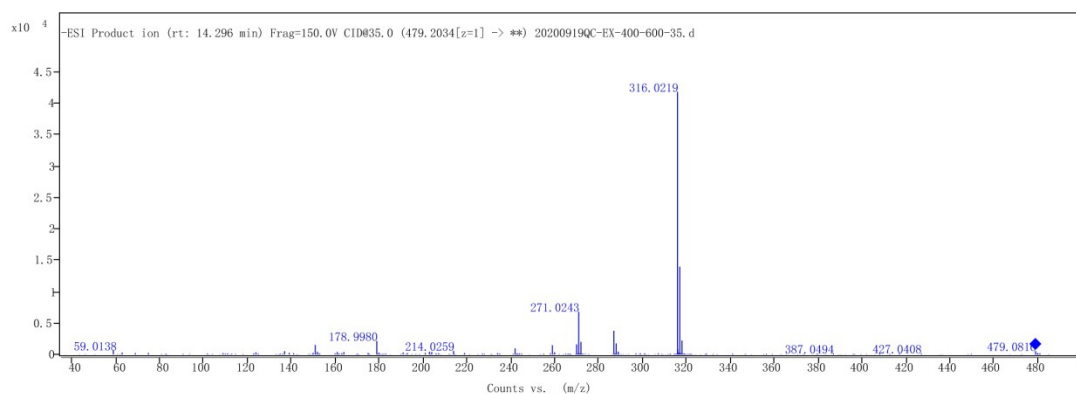
183

184 38. Compound: Myricetin-3-O-galactoside M/Z 479.0837 Formula C₂₁H₂₀O₁₃



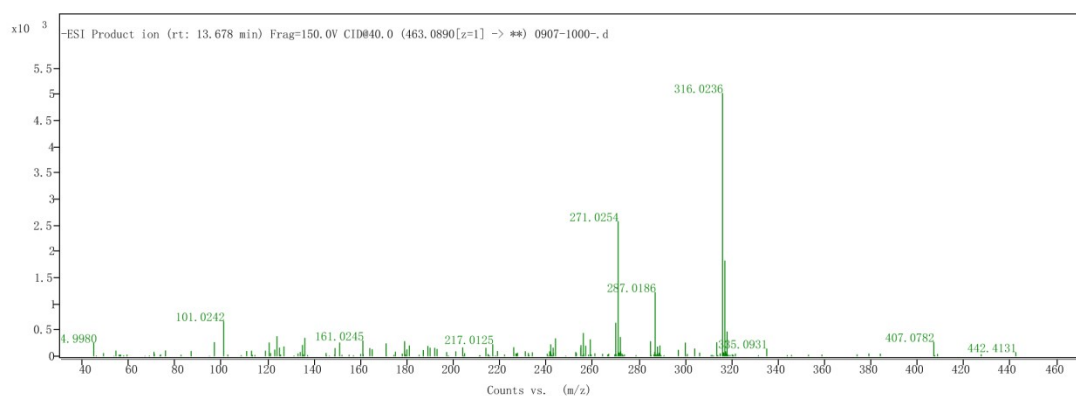
185

186 39. Compound: Quercetagitrin M/Z 479.0816 Formula C₂₁H₂₀O₁₃



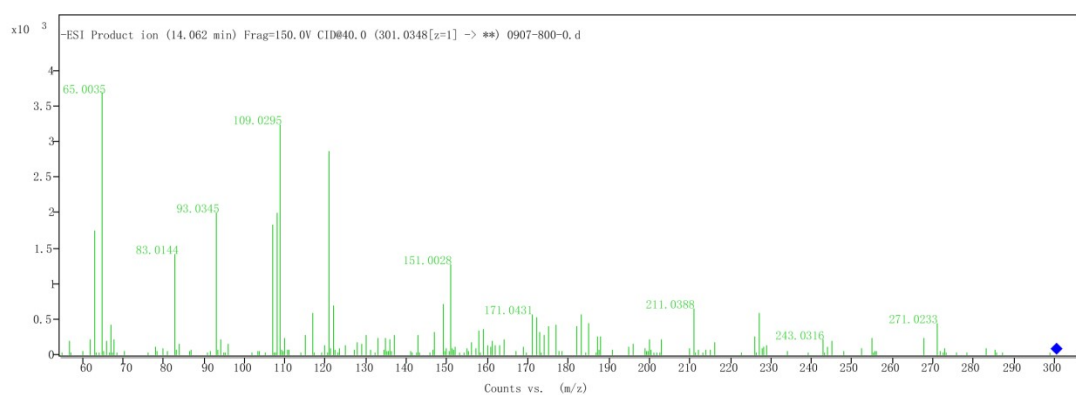
187

188 40. Compound: Myricetin-3-O-rhamnoside M/Z 463.0890 Formula C₂₁H₂₀O₁₂



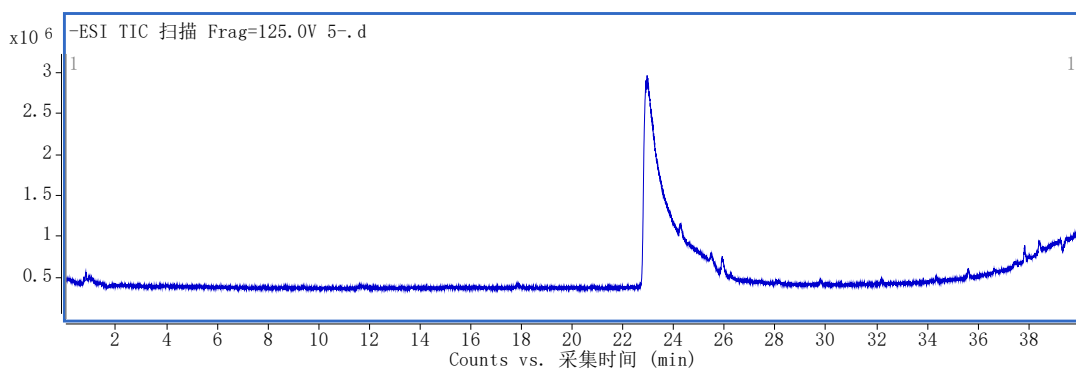
189

190 41. Compound: Quercetin M/Z 301.0348 Formula C₁₅H₁₀O₇



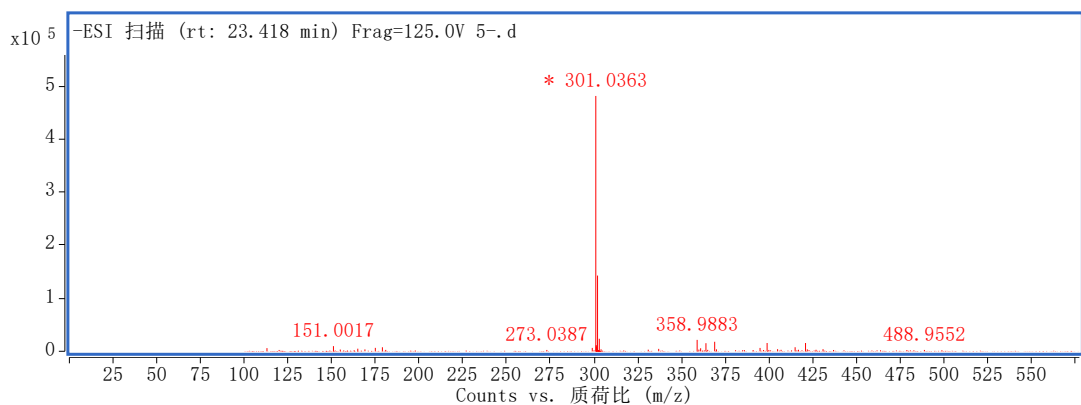
191

192 TIC of the standard

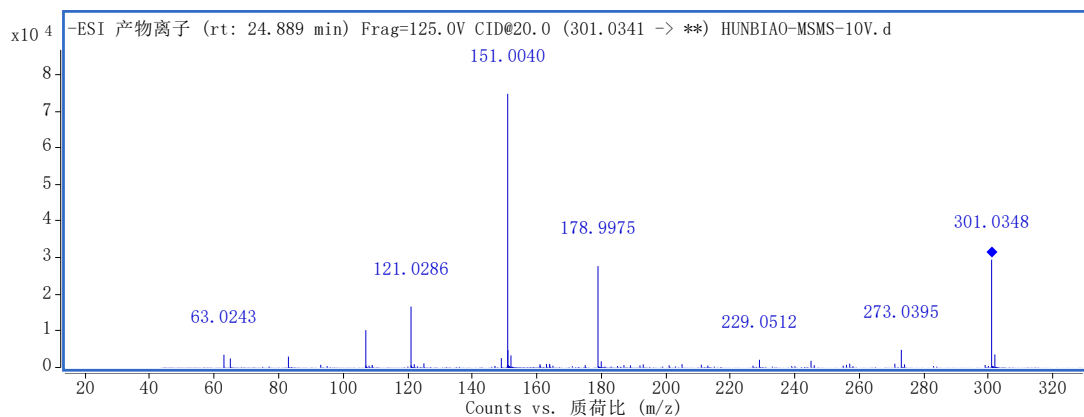


193

194 MS of the standard

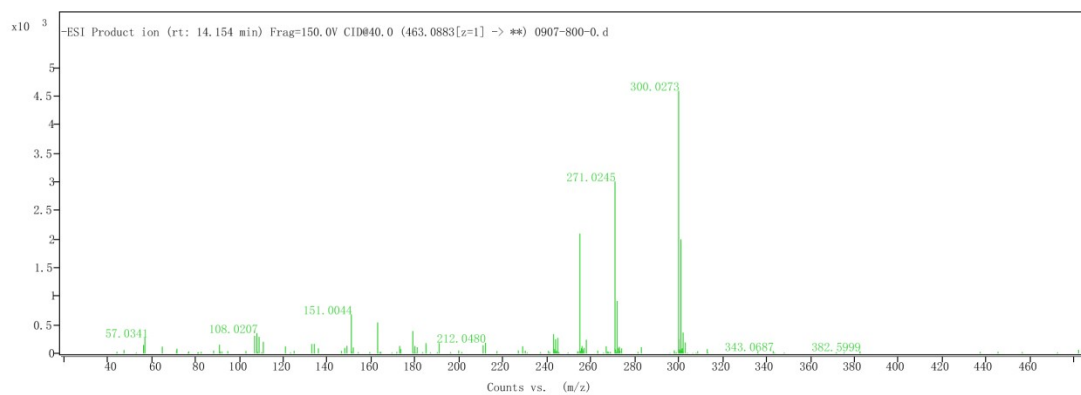


196 MS/MS of the standard



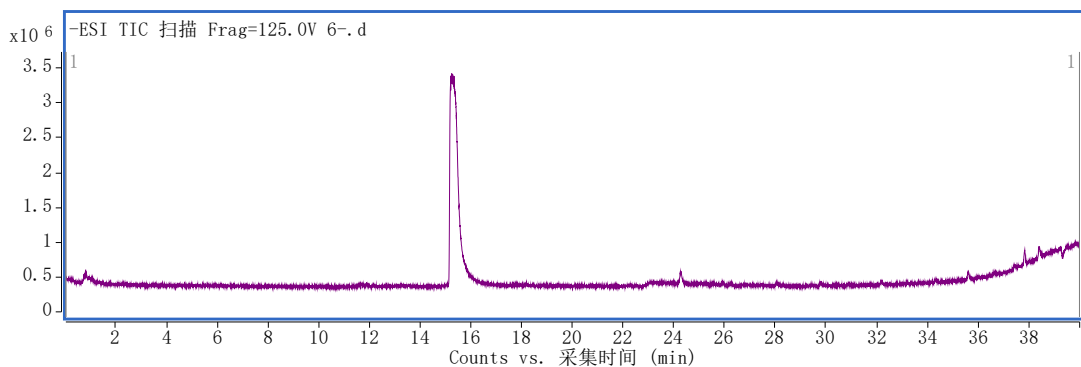
197

198 42. Compound: Quercetin-3-O-glucoside M/Z 463.0883 Formula C₂₁H₂₀O₁₂



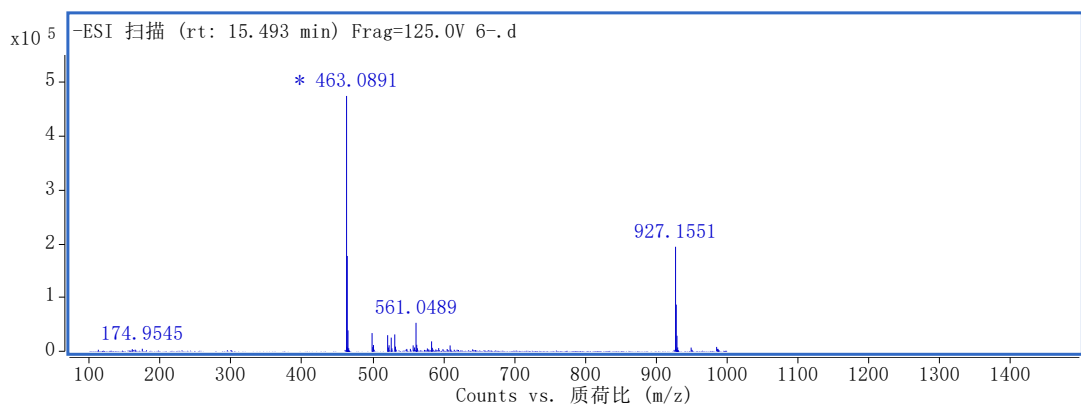
199

200 TIC of the standard

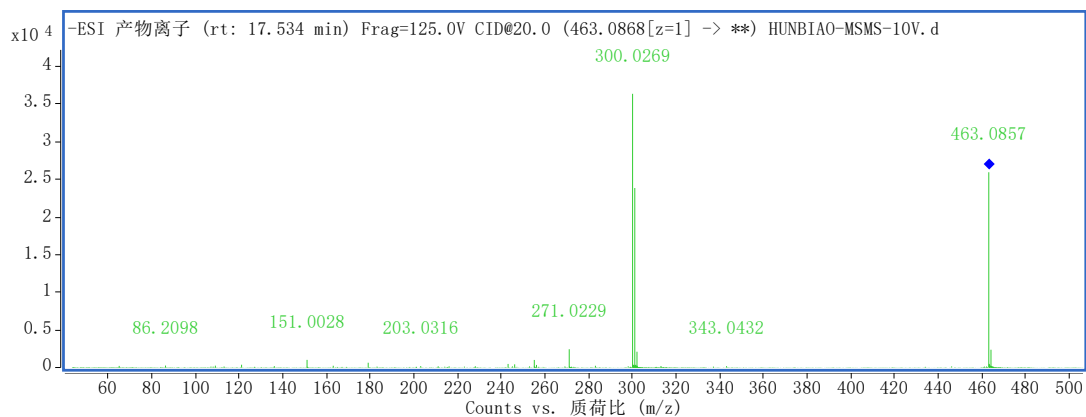


201

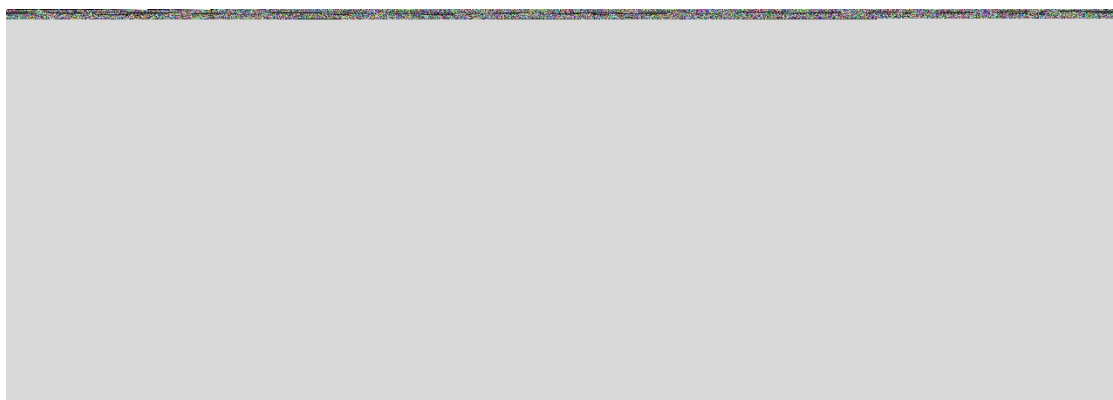
202 MS of the standard



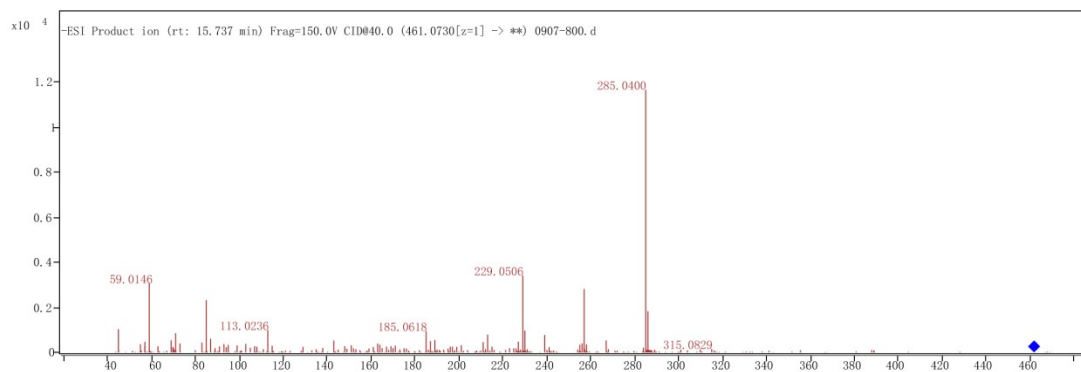
204 MS/MS of the standard



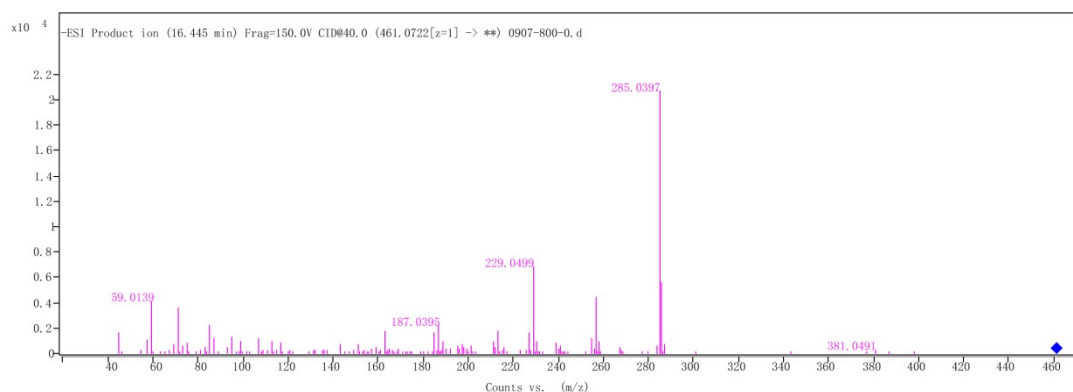
205
206 43. Compound: Quercetin 3-O-glucuronide M/Z 477.0681 Formula C₂₁H₁₈O₁₃



207
208 44. Compound: Quercetin-3-O-galactoside M/Z 463.0890 Formula C₂₁H₂₀O₁₂

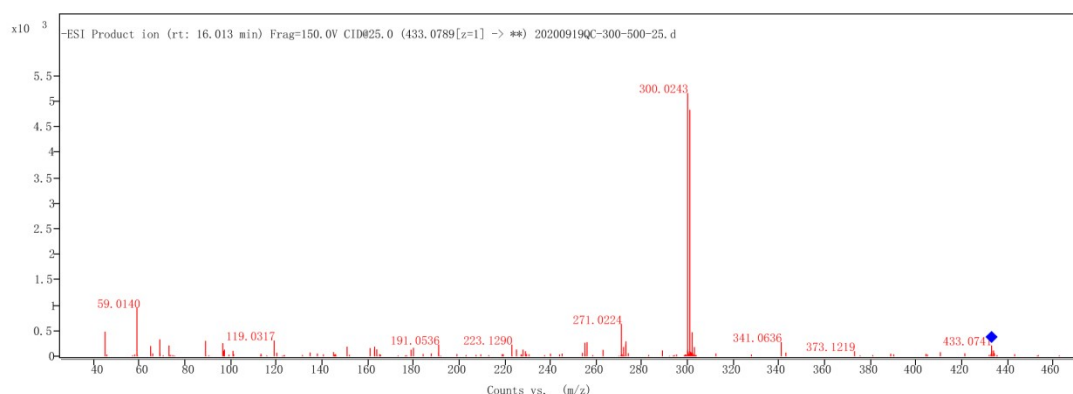


209
210 45. Compound: Luteolin-7-O-glucuronide M/Z 461.0730 Formula C₂₁H₁₈O₁₂



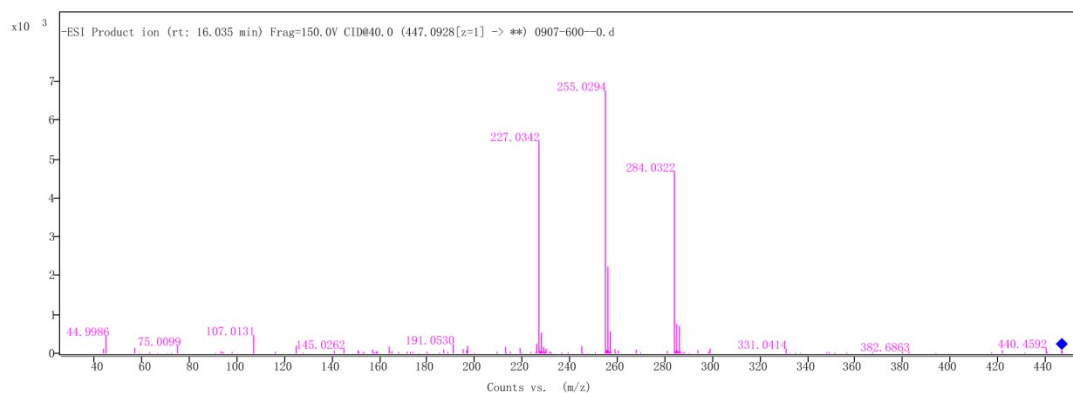
211

212 46. Compound: Avicularin M/Z 433.0789 Formula C₂₀H₁₈O₁₁



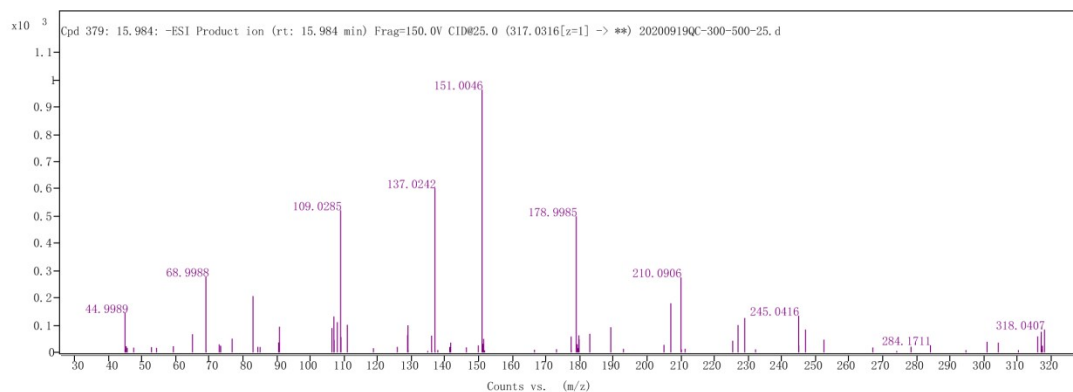
213

214 47. Compound: Kaempferol-3-O-galactoside M/Z 447.0926 Formula C₂₁H₂₀O₁₁



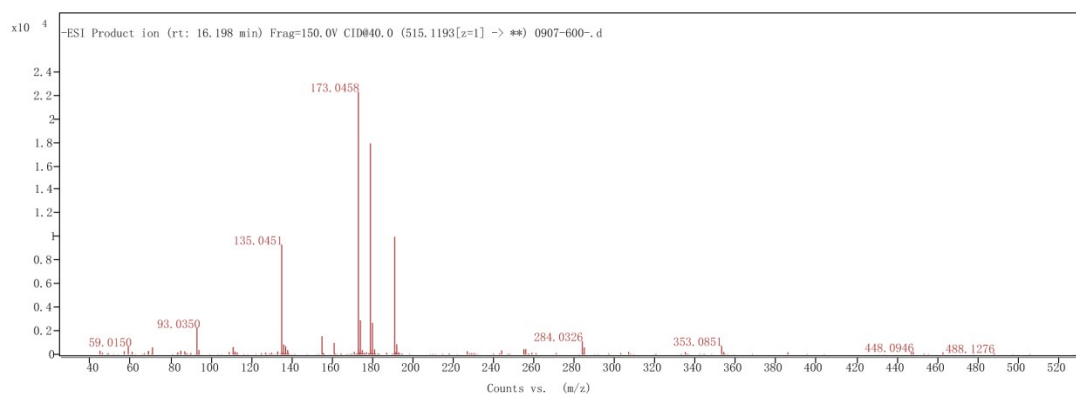
215

216 48. Compound: Myricetin M/Z 317.0316 Formula C₁₅H₁₀O₈



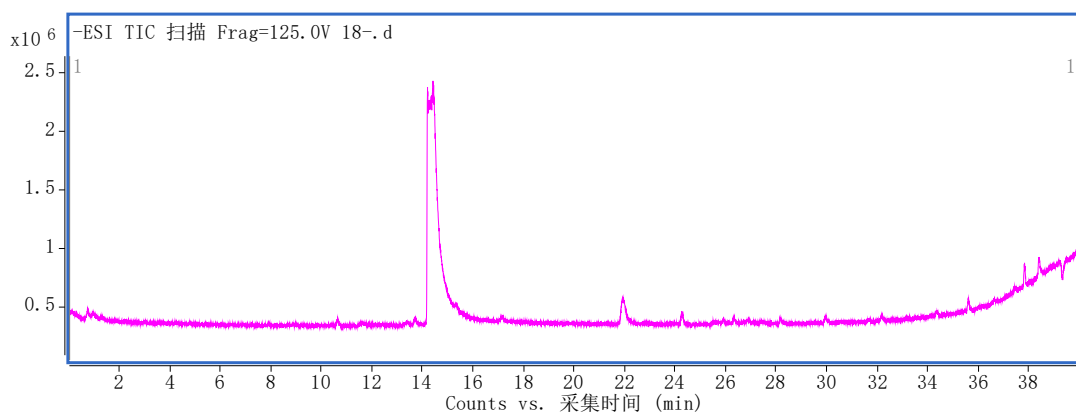
217

218 49. Compound: 3,4-Dicaffeoylquinic Acid M/Z 515.1193 Formula C₂₅H₂₄O₁₂



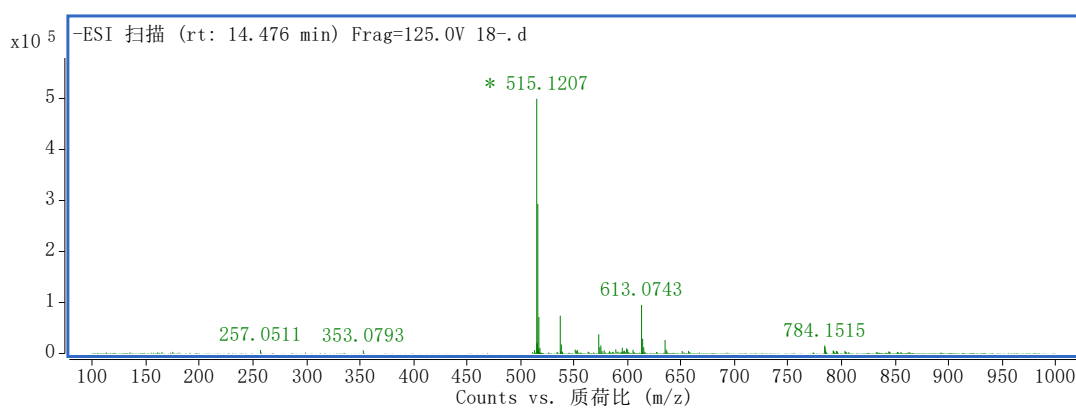
219

220 TIC of the standard



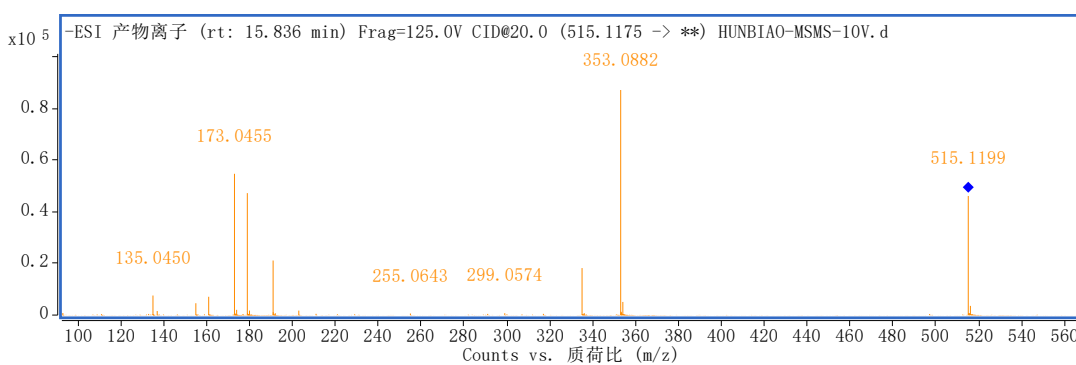
221

222 MS of the standard



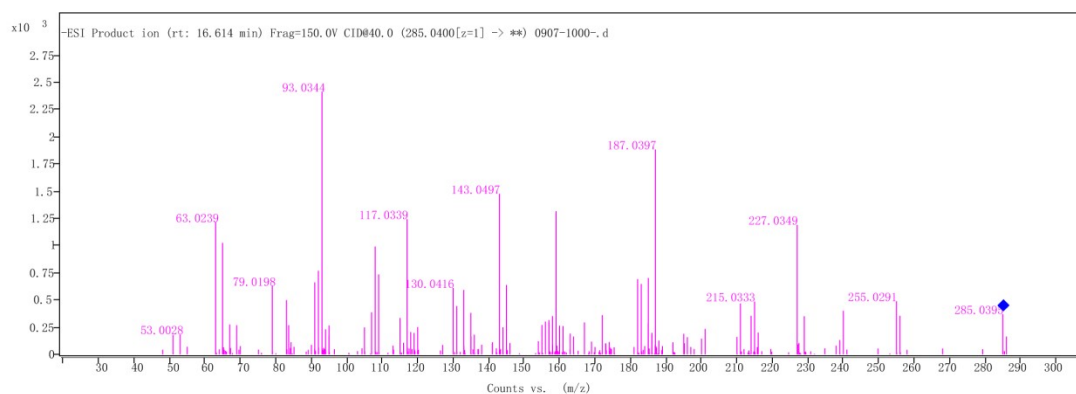
223

224 MS/MS of the standard



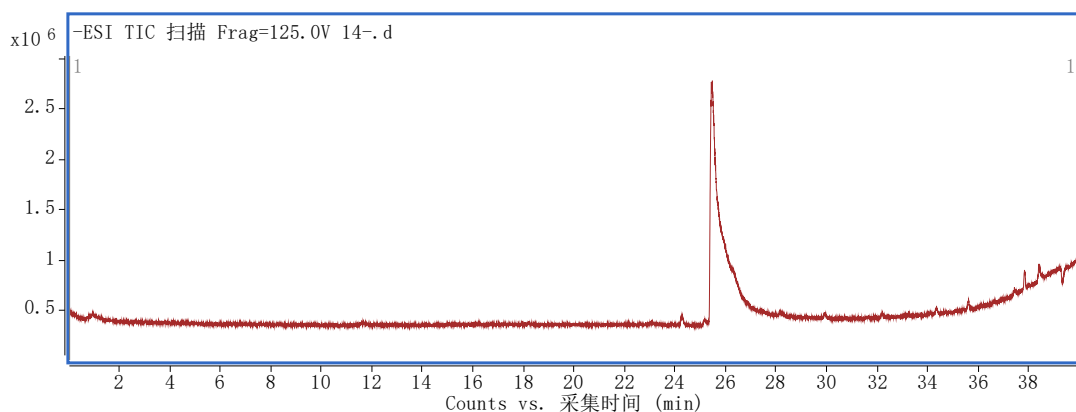
225

226 50. Compound: Kaempferol M/Z 285.0395 Formula C₁₅H₁₀O₆



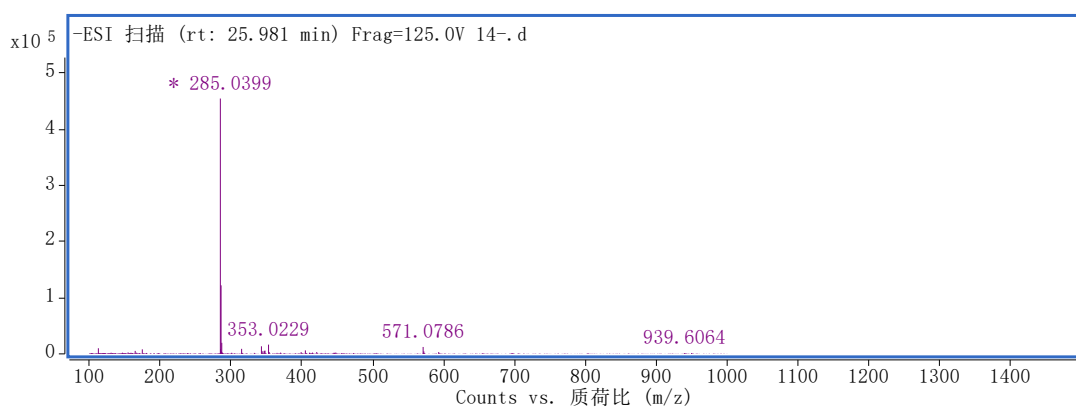
227

228 TIC of the standard



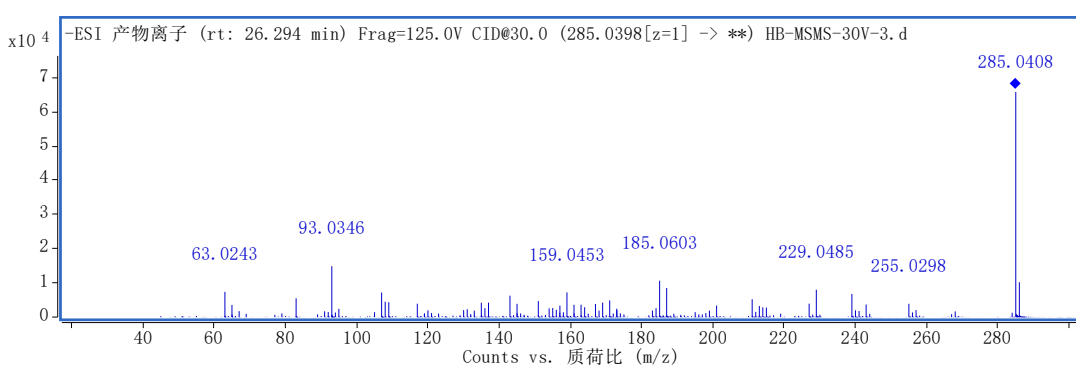
229

230 MS of the standard



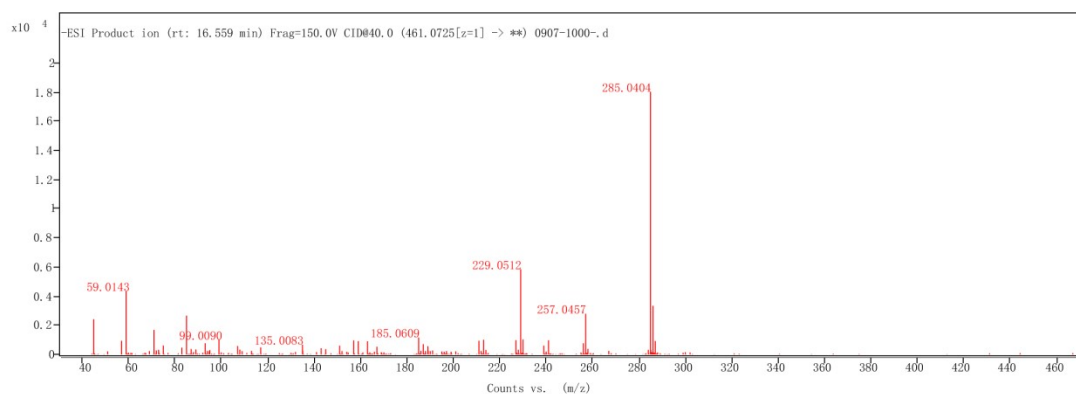
231

232 MS/MS of the standard



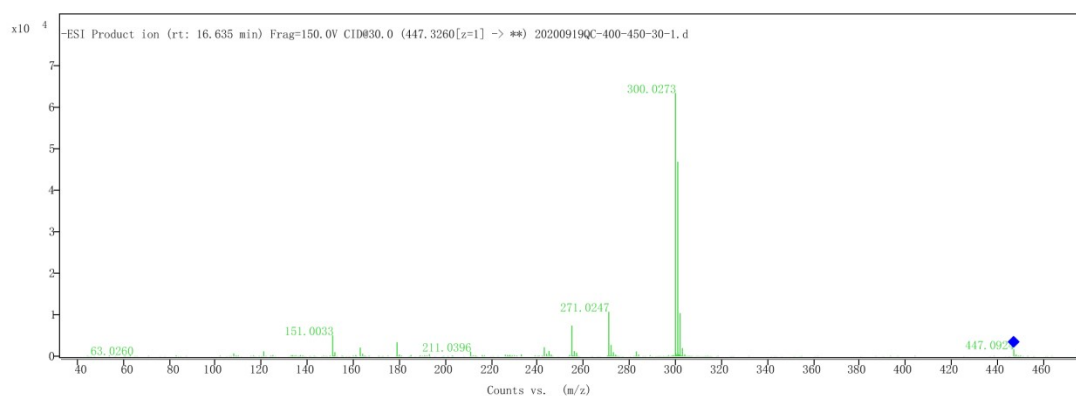
233

234 51. Compound: Kaempferol-3-O-glucuronoside M/Z 461.0731 Formula C₂₁H₁₈O₁₂



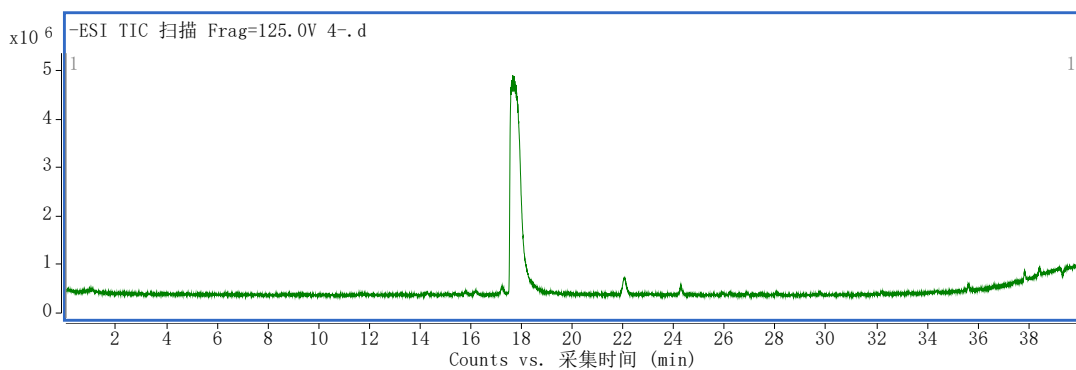
235

236 52. Compound: Quercitrin M/Z 447.0924 Formula C₂₁H₂₀O₁₁



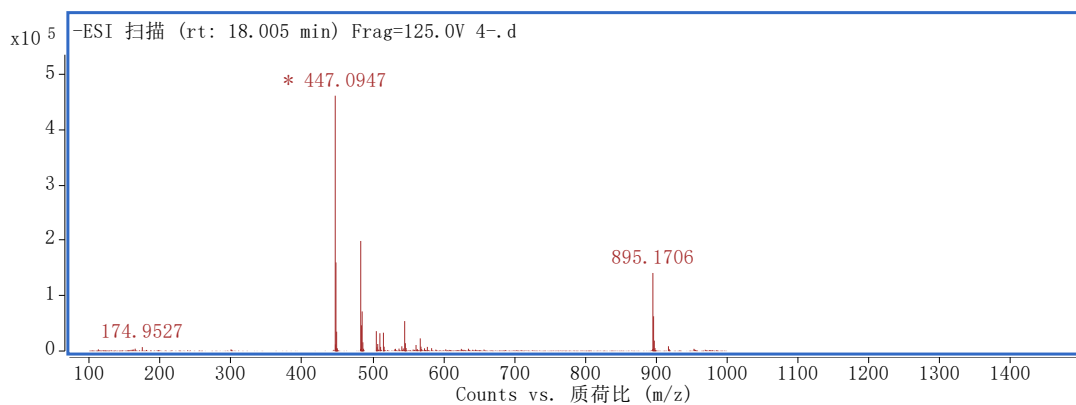
237

238 TIC of the standard



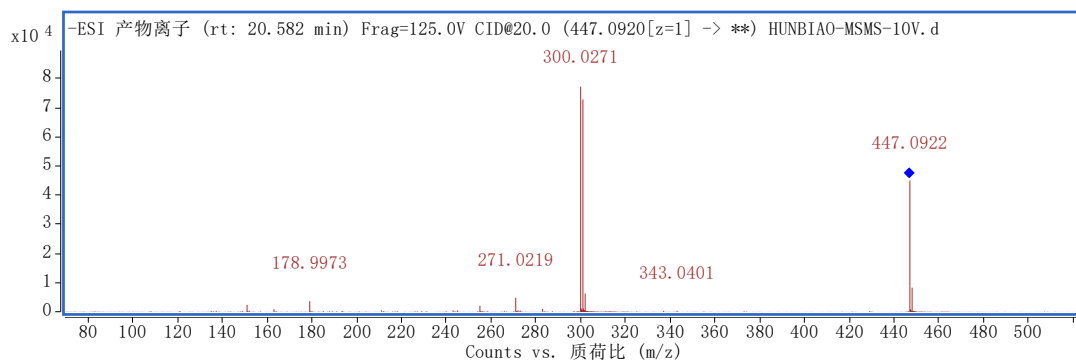
239

240 MS of the standard



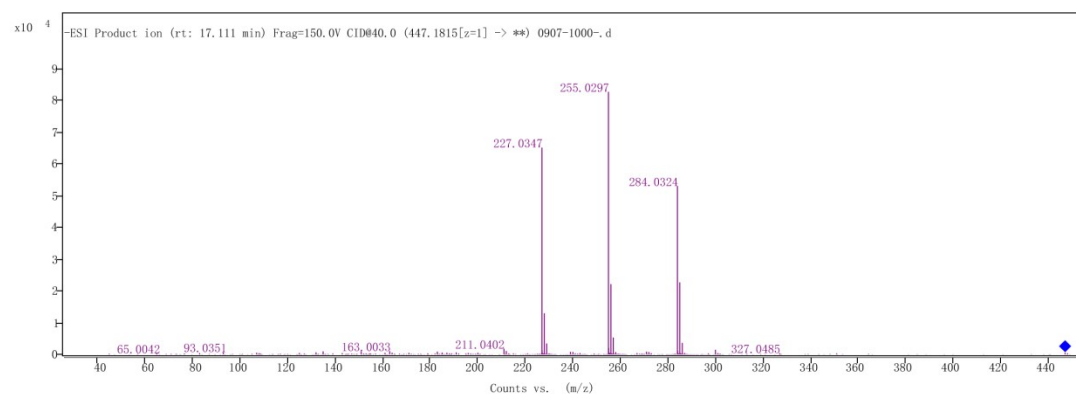
241

242 MS/MS of the standard



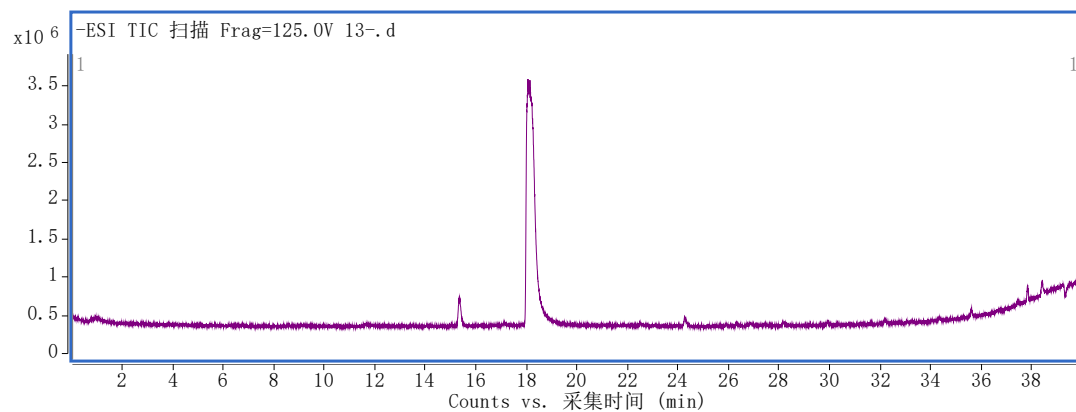
243

244 53. Compound: Kaempferol-3-O-glucoside M/Z 447.0936 Formula C₂₁H₂₀O₁₁



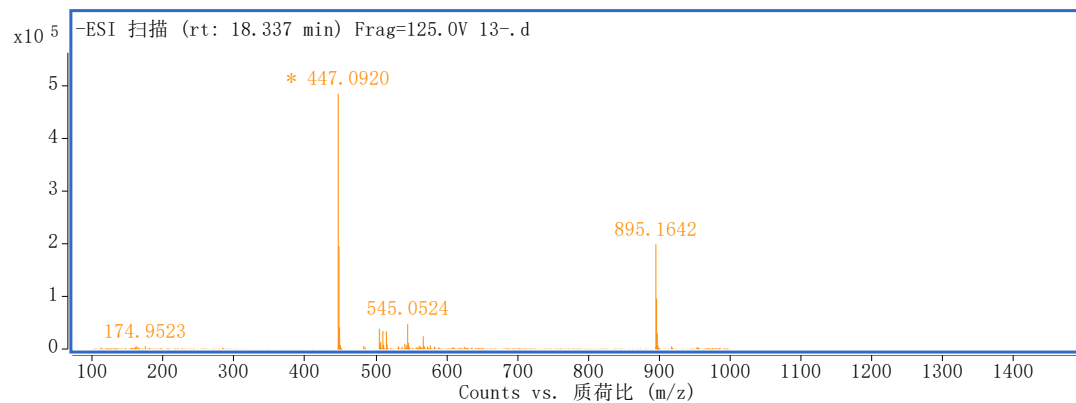
245

246 TIC of the standard



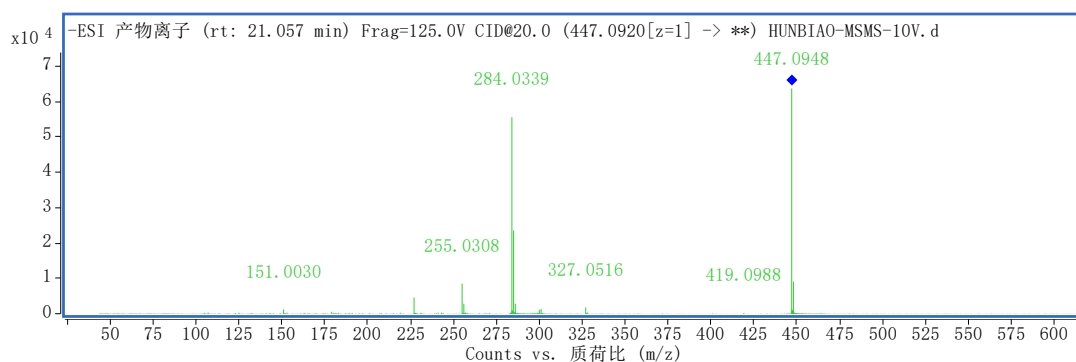
247

248 MS of the standard



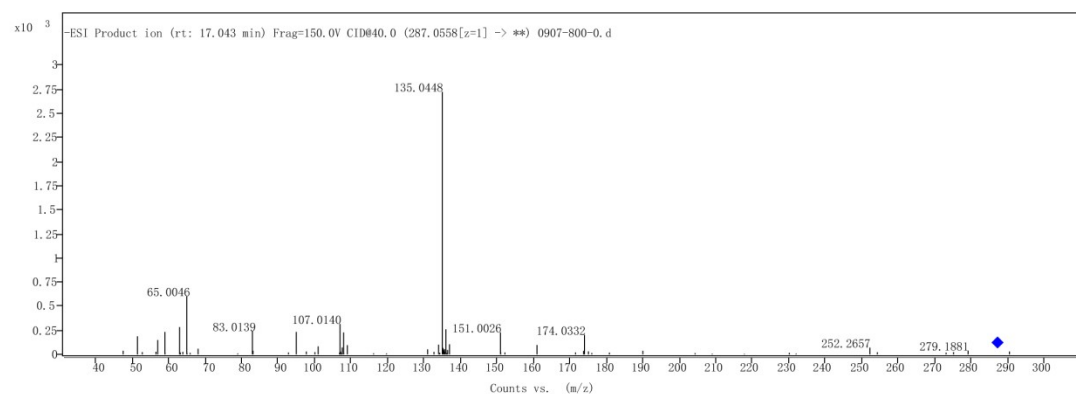
249

250 MS/MS of the standard



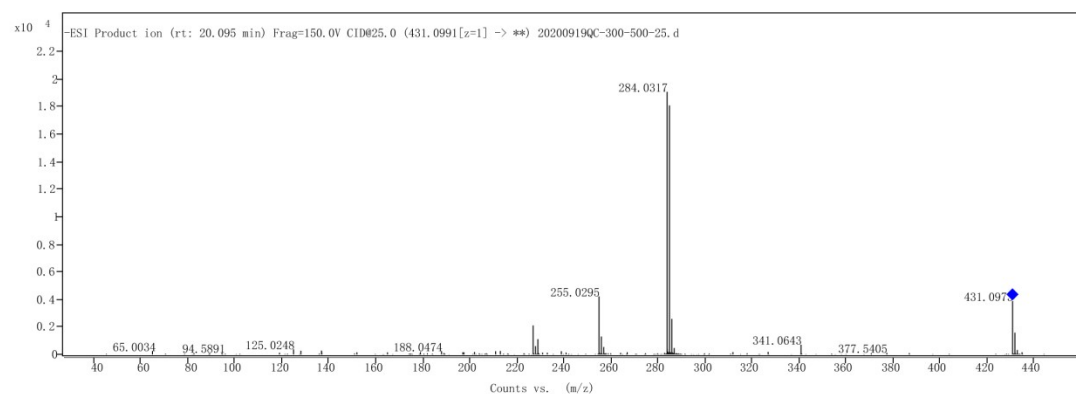
251

252 54. Compound: Eriodicryol M/Z 287.0558 Formula C₁₅H₁₂O₆



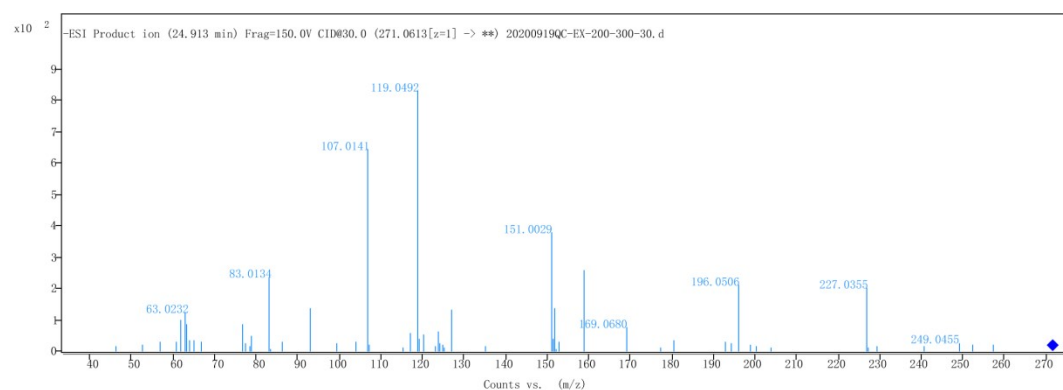
253

254 55. Compound: Kaempferol-3-rhamnoside M/Z 431.0973 Formula C₂₁H₂₀O₁₀



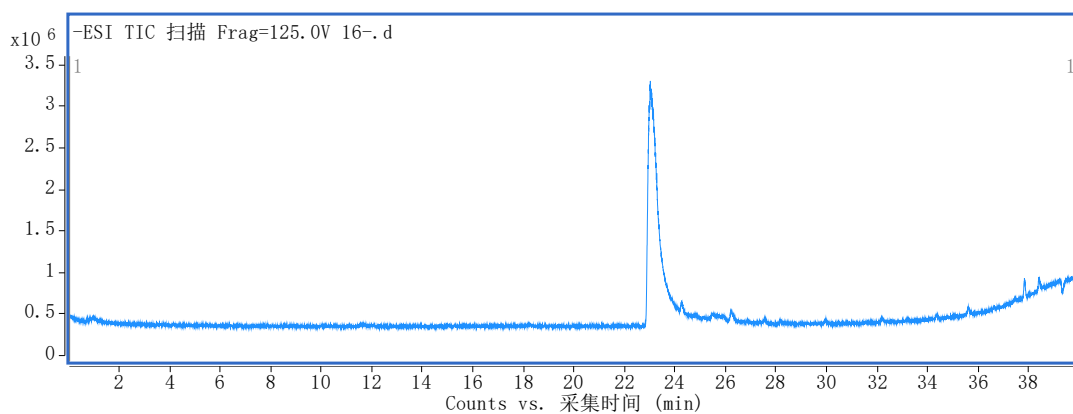
255

256 56. Compound: Naringenin M/Z 271.0603 Formula C₁₅H₁₂O₅



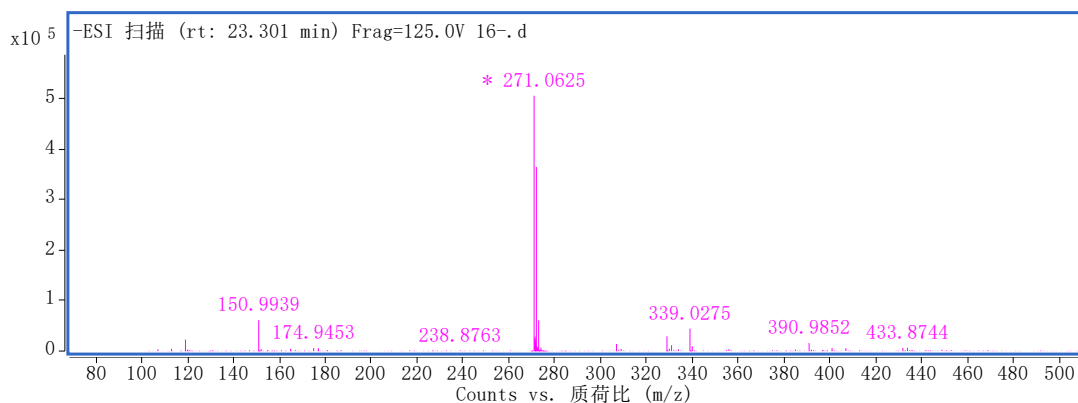
257

258 TIC of the standard



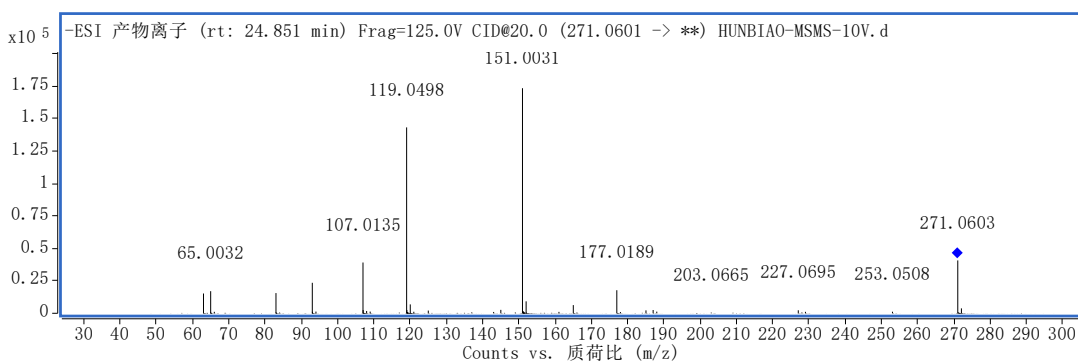
259

260 MS of the standard



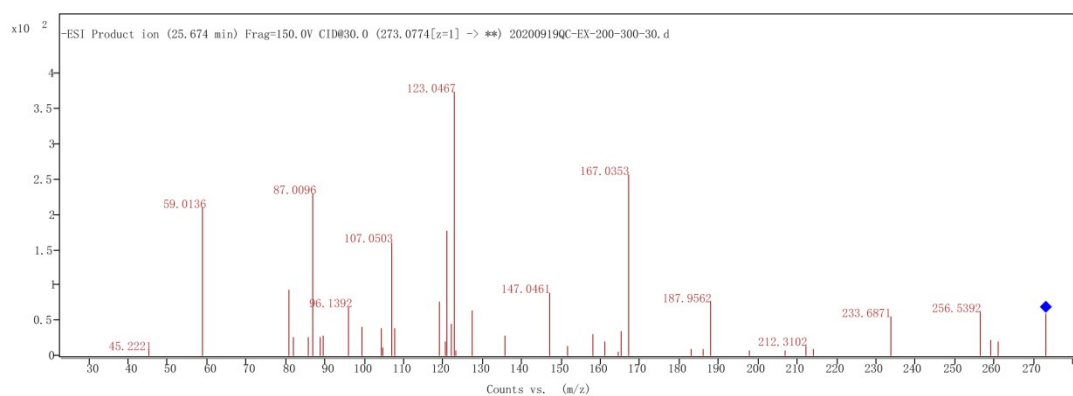
261

262 MS/MS of the standard



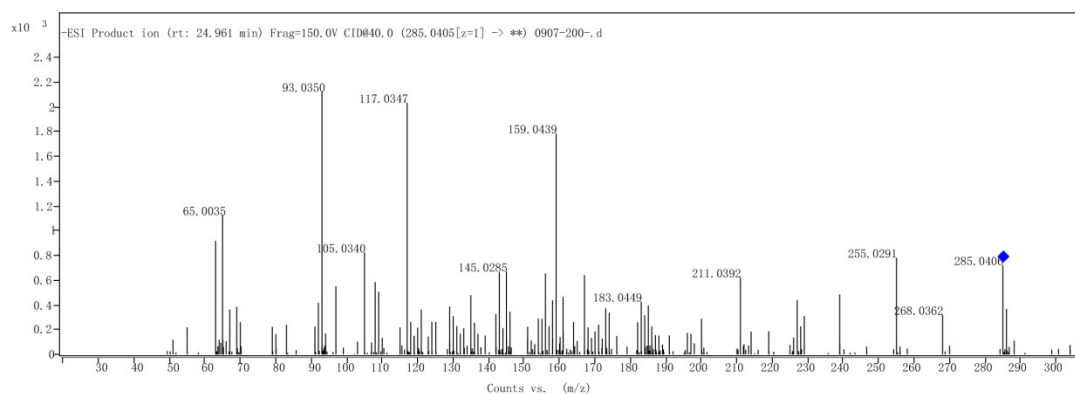
263

264 57. Compound: Phloretin M/Z 273.0768 Formula C₁₅H₁₄O₅



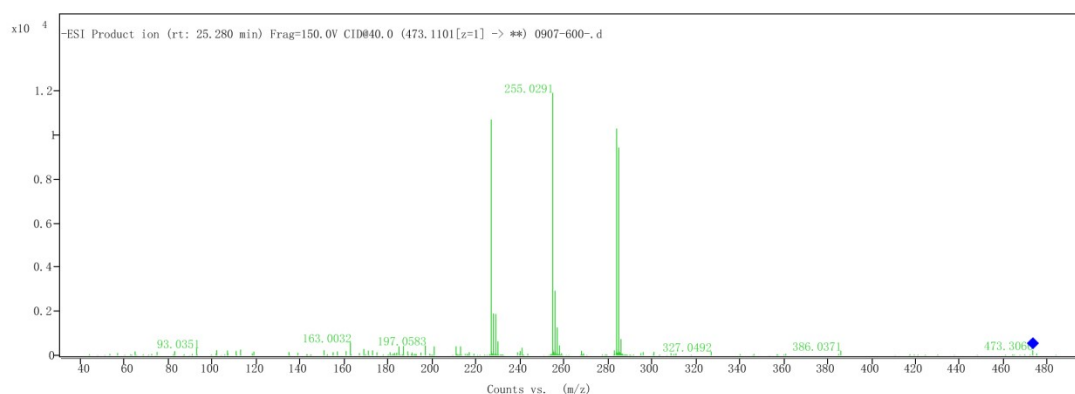
265

266 58. Compound: Luteolin M/Z 285.0406 Formula C₁₅H₁₀O₆



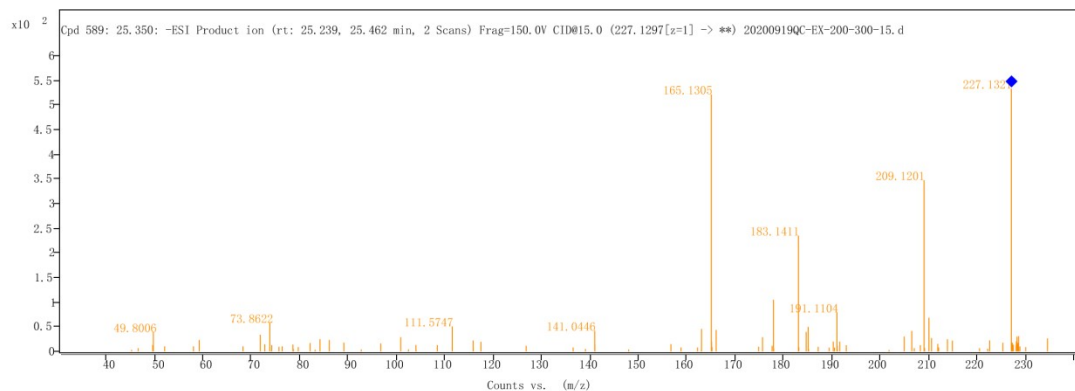
267

268 59. Compound: Kaempferol-3-(2''-acetylramnoside) M/Z 473.1101 Formula
269 C₂₃H₂₂O₁₁



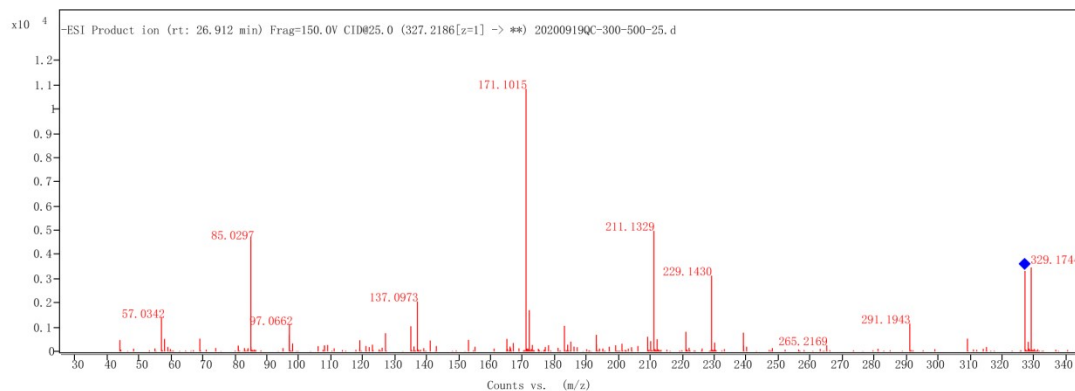
270

271 60. Compound: Traumatic Acid M/Z 227.1297 Formula C₁₂H₂₀O₄



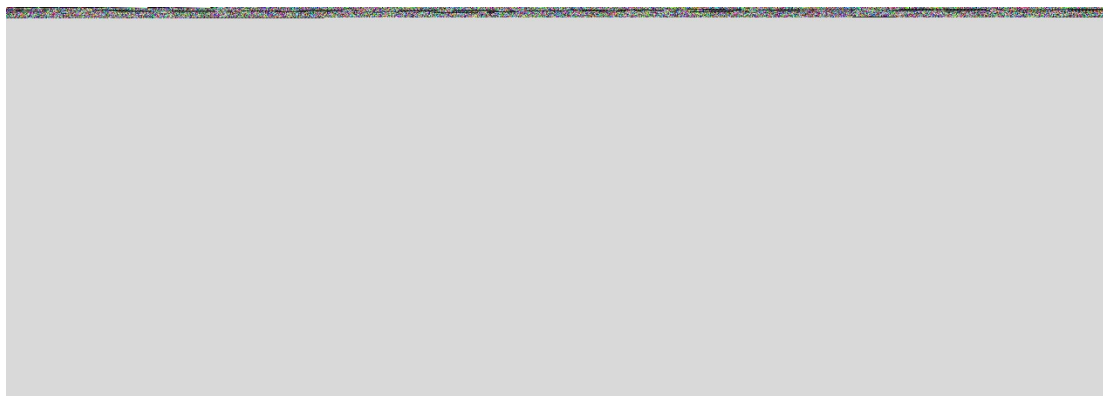
272

273 61. Compound: Trihydroxyoctadecadienoic acid M/Z 327.2186 Formula C₁₈H₃₂O₅



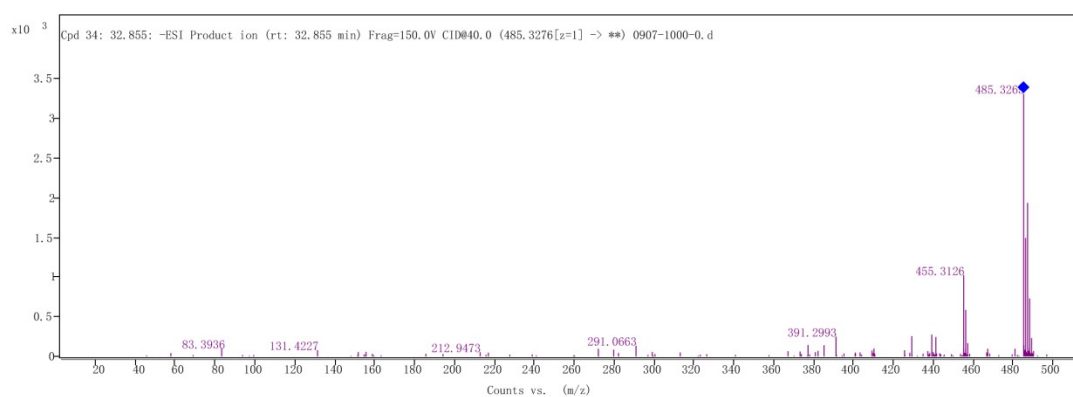
274

275 62. Compound: Kaempferol-3-(6''-(Z)-Cinnamyl)glucoside M/Z 577.1357 Formula
276 C₃₀H₂₆O₁₂



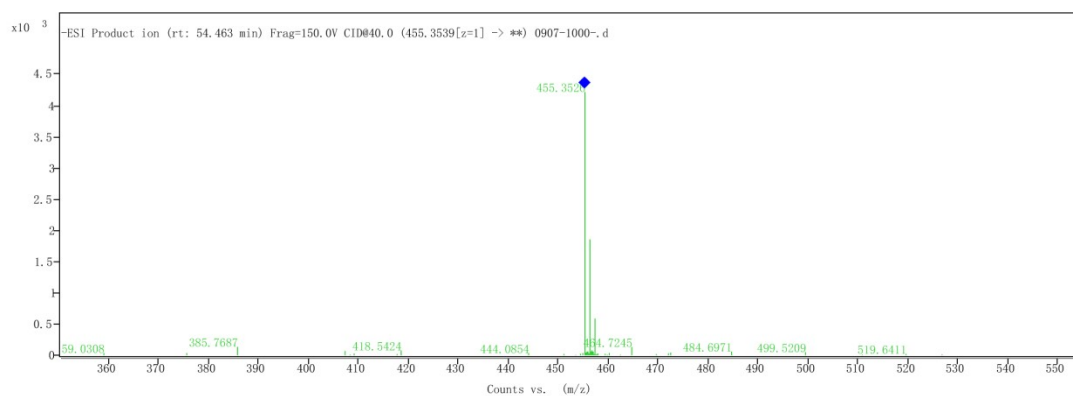
277

278 63. Compound: Cyclocaric acid B M/Z 485.3265 Formula C₃₀H₄₆O₅



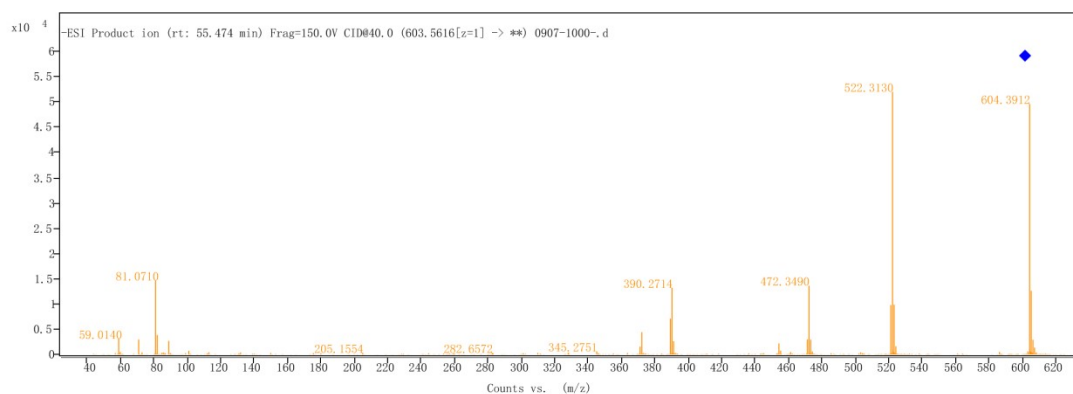
279

280 64. Compound: Ursolic acid M/Z 455.3526 Formula C₃₀H₄₈O₃



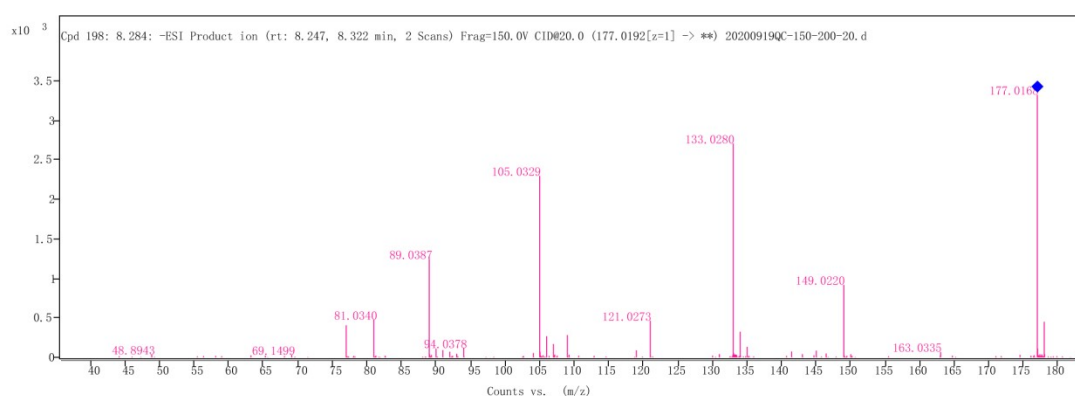
281

282 65. Compound: Hederagenin-3-O-arabinoside M/Z 603.3912 Formula C₃₅H₅₆O₈



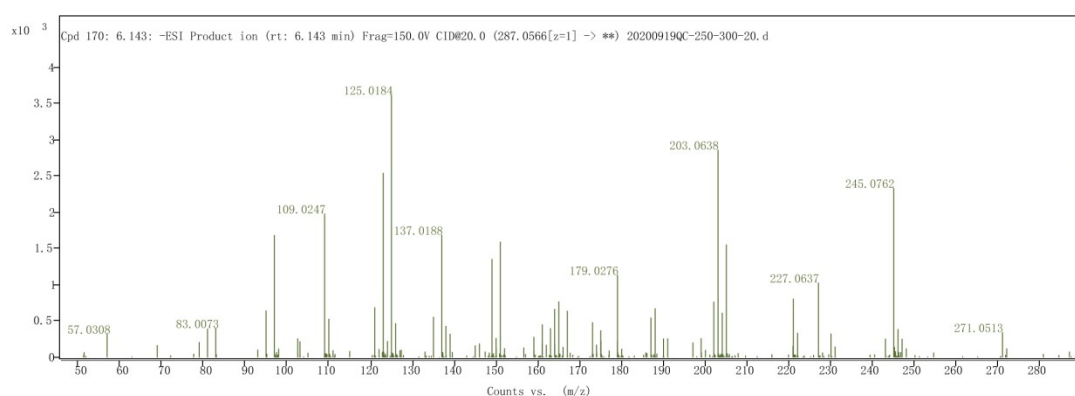
283

284 66. Compound: Esculetin M/Z 177.0192 Formula C₉H₆O₄



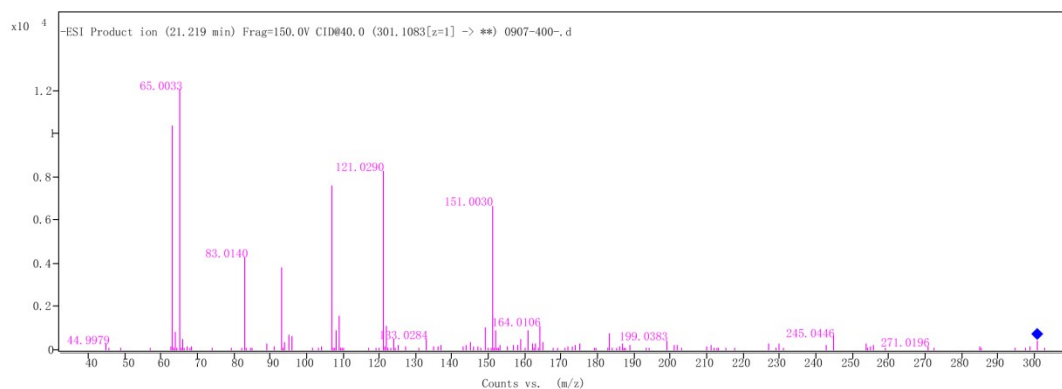
285

286 67. Compound: Dihydrokaempferol M/Z 287.0566 Formula C₁₅H₁₂O₆



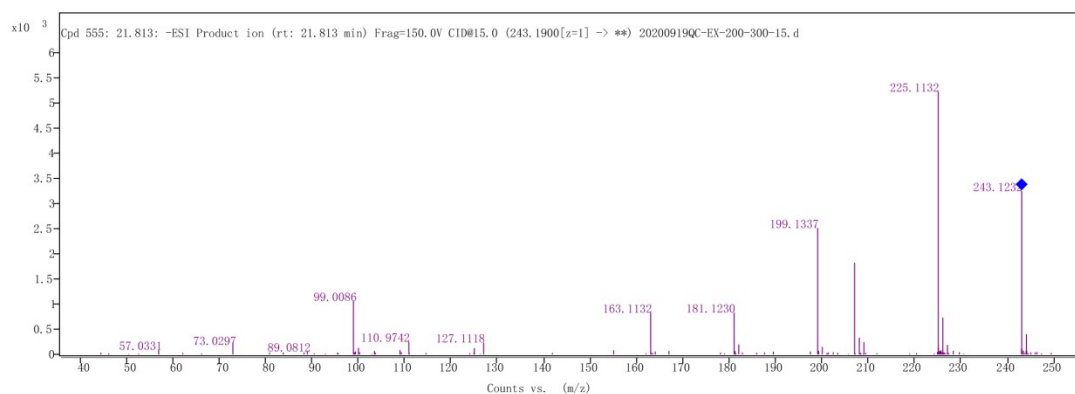
287

288 68. Compound: Hieracin M/Z 301.0343 Formula C₁₅H₁₀O₇



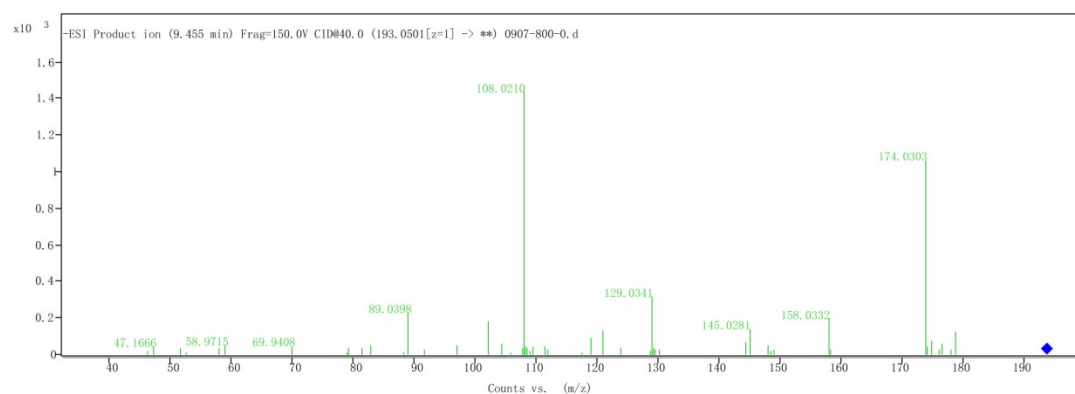
289

290 69. Compound: 4-Oxododecanedioic acid M/Z 243.1232 Formula C₁₂H₂₀O₅



291

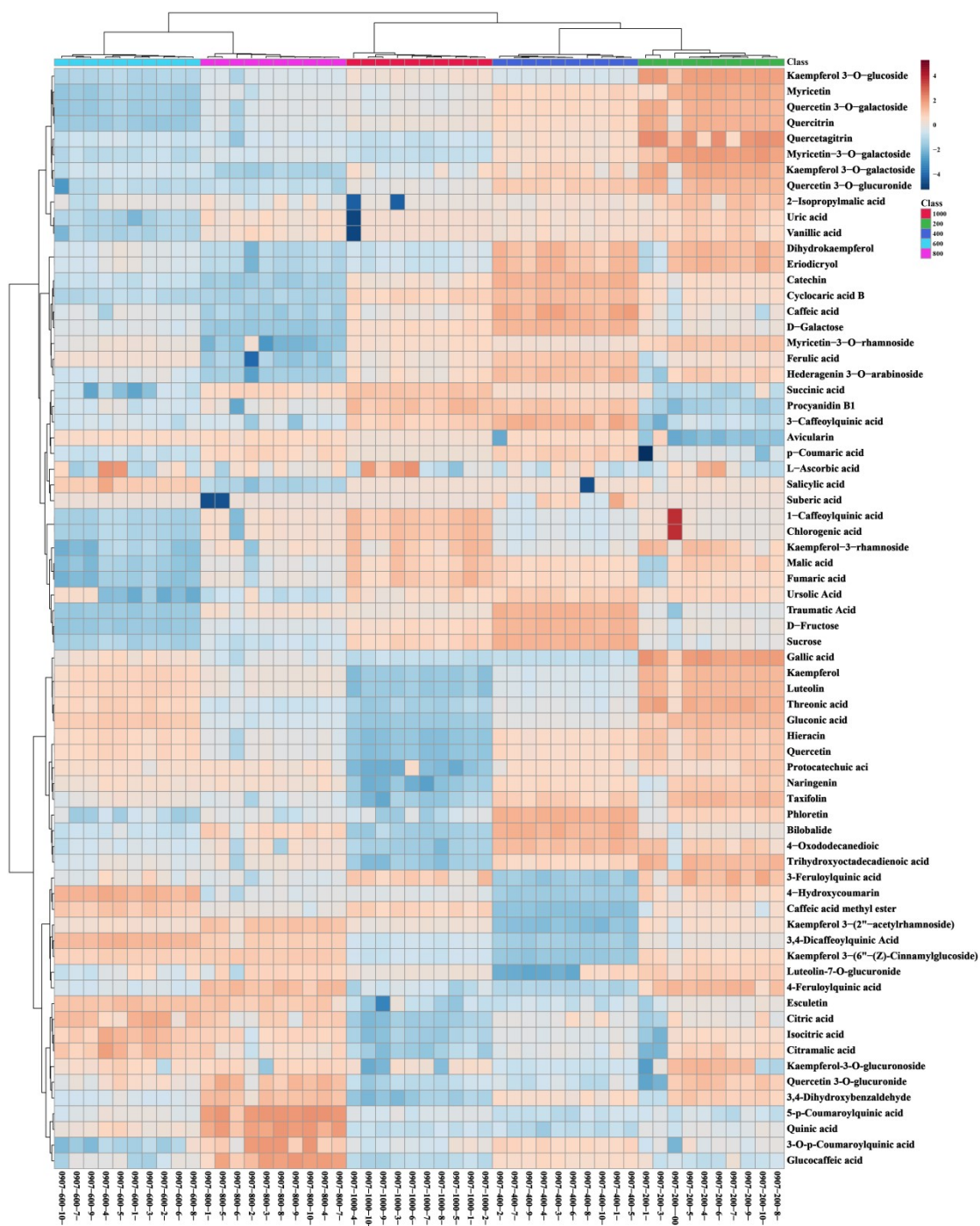
292 70. Compound: Caffeic acid methyl ester M/Z 193.0504 Formula C₁₀H₁₀O₄



293

294

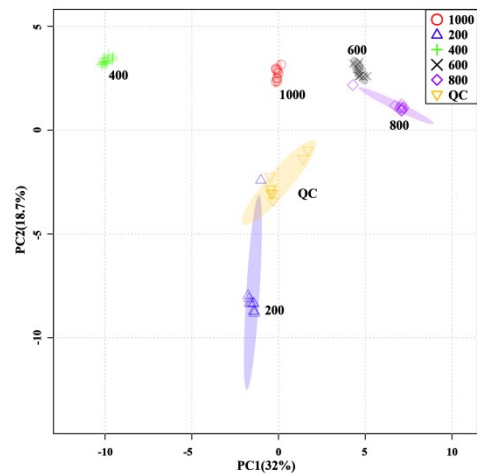
295 ● Heatmap of 70 differential metabolites (Fig. S4)



296

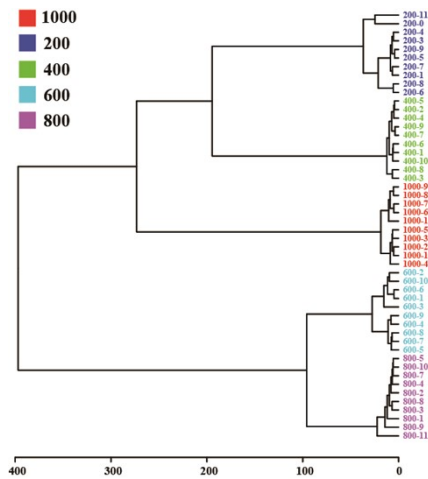
297

298 ● QC sample were clustered in the center of the PCA plot (Fig. S5).



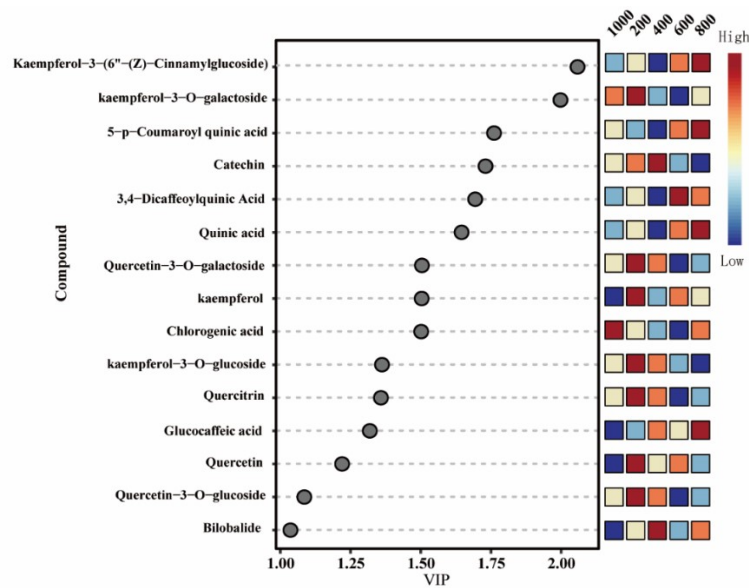
299

300 ● Cluster dendrogram of the data set concluded for five different altitude environments
301 of *C. paliurus* leaves (Fig. S6).



302

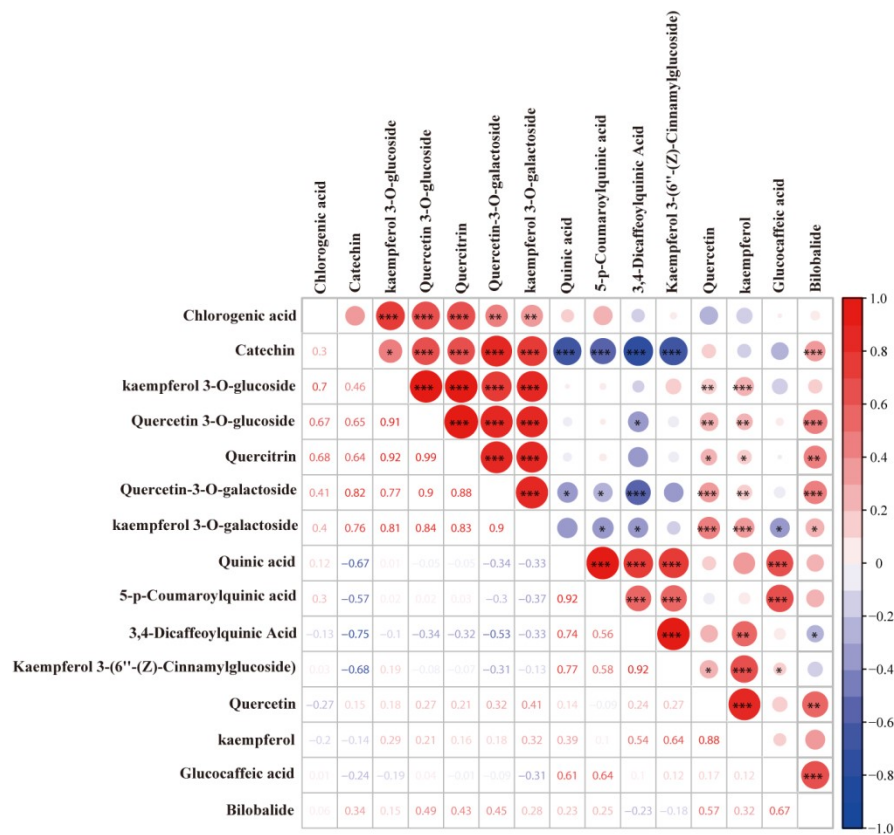
303 ● Variable importance on projection (VIP) scores from the PLS-DA model indicating the
304 most discriminating metabolites among *C. paliurus* leaves from different altitude
305 environments in descending order of importance with relative levels of the metabolite
306 (Fig. S7).



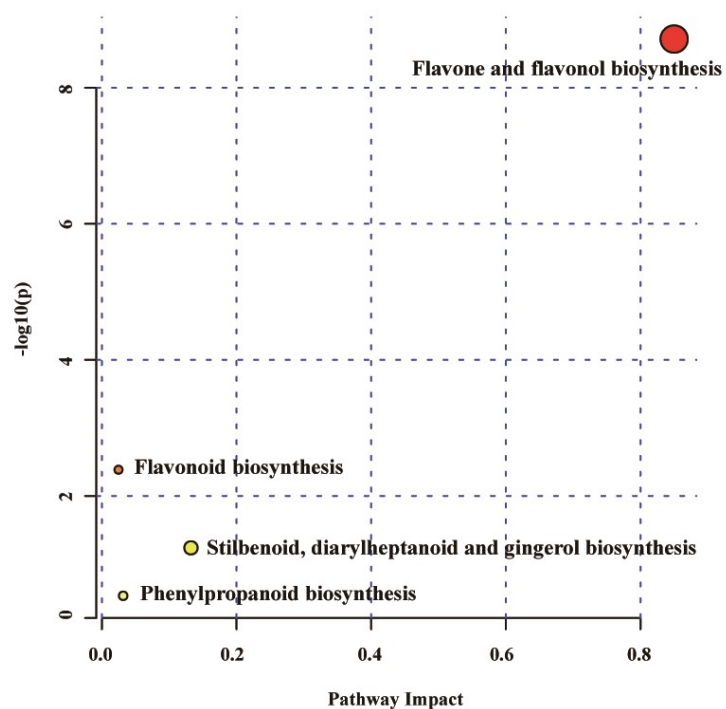
307

308

309 ● Correlation analysis heatmap of fifteen metabolites with VIP > 1.0 and P < 0.05 (*P < 0.05,
310 **P < 0.01, ***P < 0.001) (Fig. S8).



313 ● Pathway topology analysis related with differential metabolites (Fig. S9).



314

Pathway Name	Match Status	p	$-\log(p)$	Holm p	FDR	Impact
Flavone and flavonol biosynthesis	5/10	1.9279E-9	8.7149	1.8508E-7	1.8508E-7	0.85000
Flavonoid biosynthesis	3/47	0.0041204	2.3851	0.39144	0.19778	0.02471
Stilbenoid, diarylheptanoid and gingerol biosynthesis	1/8	0.0579550	1.2369	1.0	1.0	0.13235
Phenylpropanoid biosynthesis	1/46	0.2937600	0.53201	1.0	1.0	0.03161

316 ● The information concerning the identification of compounds (Table S1).

NO	RT ^a	Proposed compound	M/Z ^b	M/Z ^c	Error (ppm)	Elemental composition	Classification	M/Z (Fragment ion)
1	0.81	Threonic acid	135.0303	135.0299	2.96	C ₄ H ₈ O ₅	others	117.0196,75.0094,59.0142
2	0.86	D-Fructose	179.0555	179.0561	-3.35	C ₆ H ₁₂ O ₆	carbohydrates	89.0140,71.0149,59.0148
3	1.05	Fumaric acid	115.0034	115.0037	-2.61	C ₄ H ₄ O ₄	others	71.0143,73.0302,59.0153,44.0230
4	1.09	Quinic acid	191.0565	191.0561	2.09	C ₇ H ₁₂ O ₆	others	111.0092,93.0351,87.0094,85.0301,67.0195,57.0352
5	1.10	*Malic acid	133.0141	133.0142	-0.75	C ₄ H ₆ O ₅	others	115.0022,89.0234,71.0125,72.9928,44.9978
6	1.11	Gluconic acid	195.0505	195.0510	-2.56	C ₆ H ₁₂ O ₇	others	129.0200,99.0089,87.0089,75.0091,71.0144,59.0146
7	1.25	D-Galactose	179.0562	179.0561	0.56	C ₆ H ₁₂ O ₆	carbohydrates	87.0088,71.0139,59.0144,55.0186
8	1.28	Sucrose	341.1090	341.1089	0.29	C ₁₂ H ₂₂ O ₁₁	carbohydrates	179.0558,101.0252,89.0251,71.0136,59.0140
9	1.30	Uric acid	167.0206	167.0211	-2.75	C ₅ H ₄ N ₄ O ₃	others	124.01675,96.02182,69.01030,
10	1.39	Isocitric acid	191.0190	191.0197	-3.82	C ₆ H ₈ O ₇	others	129.0188,111.0087,87.0091,85.0299,67.0188
11	1.40	*Citric acid	191.0192	191.0197	-2.77	C ₆ H ₈ O ₇	others	129.0188,111.0084,87.0089,85.0296,67.0189
12	1.73	*Succinic acid	117.0188	117.0193	-4.27	C ₄ H ₆ O ₄	others	99.9264,73.0300
13	1.74	Citramalic acid	147.0297	147.0299	-1.56	C ₅ H ₈ O ₅	others	129.02001,101.02346,85.02832,
14	2.23	*Gallic acid	169.0134	169.0142	-4.73	C ₇ H ₆ O ₅	phenolic acids	143.0742,125.0237,97.0284,81.0342,54.0403
15	3.33	*Vanillic acid	167.0358	167.0350	4.67	C ₈ H ₈ O ₄	phenolic acids	152.01356,108.02316
16	4.00	*Protocatechuic acid	153.0189	153.0193	-2.61	C ₇ H ₆ O ₄	phenolic acids	109.0298,108.0221,91.0292,81.0340
17	4.67	4-Caffeoylquinic acid	353.0875	353.0878	-0.85	C ₁₆ H ₁₈ O ₉	phenolic acids	191.0554,179.0343,135.0448
18	4.73	Salicylic acid	137.0239	137.0244	-3.65	C ₇ H ₆ O ₃	phenolic acids	93.0344,65.0401,45.2489
19	4.92	Procyanidin B1	577.1331	577.1351	-3.47	C ₃₀ H ₂₆ O ₁₂	dimeric/trimeric catechins	408.0811,289.0704,125.0247
20	5.03	4-Hydroxycoumarin	161.0243	161.0244	-0.62	C ₉ H ₆ O ₃	others	132.0216,117.0338,89.0395,79.0192,51.0244
21	5.92	Glucocaffeic acid	341.0877	341.0878	-0.29	C ₁₅ H ₁₈ O ₉	carbohydrates	161.0225,135.0430,59.0135
22	6.14	Dihydrokaempferol	287.0566	287.0561	1.74	C ₁₅ H ₁₂ O ₆	flavonol and flavonol/flavone glycosides	271.0196,245.0446,183.0447,151.0030,121.0290,107.0134,93.0342
23	6.27	3,4-Dihydroxybenzaldehyde	137.0245	137.0246	-0.44	C ₇ H ₆ O ₃	others	108.0224,93.0360,81.0349,65.0377
24	6.72	L-Ascorbic acid	175.0251	175.0248	1.71	C ₆ H ₈ O ₆	others	115.0031,87.0083,71.0132,59.0134
25	6.80	Chlorogenic acid	353.0890	353.0878	3.40	C ₁₆ H ₁₈ O ₉	phenolic acids	191.0548,161.0231,93.0341,
26	7.08	3-Feruloylquinic acid	367.1037	367.1035	0.54	C ₁₇ H ₂₀ O ₉	phenolic acids	193.0490,191.0553,134.0372
27	7.40	1-Caffeoylquinic acid	353.0890	353.0878	3.40	C ₁₆ H ₁₈ O ₉	phenolic acids	191.0557,179.0345,173.0451,135.0450

28	7.46	*Caffeic acid	179.0349	179.0350	-0.56	C ₉ H ₈ O ₄	phenolic acids	135.0465,117.0355,107.0512,79.0562
29	7.66	Bilobalide	325.0930	325.0929	0.31	C ₁₅ H ₁₈ O ₈	Terpenes	145.0285,133.0637,117.0337,71.0133,59.0138
30	7.97	2-Isopropylmalic acid	175.0605	175.0612	-4.00	C ₇ H ₁₂ O ₅	others	115.0392,113.0590,85.0651,131.0695,59.0140,
31	8.28	Esculetin	177.0192	177.0193	-0.56	C ₉ H ₆ O ₄	others	149.0220,133.0280,121.0273,105.0329,89.0387,8 1.0340
32	8.64	*Catechin	289.0718	289.0718	0.00	C ₁₅ H ₁₄ O ₆	flavan-3-ols	245.0817,221.0816,203.0706,151.0386,137.0247, 109.0286
33	8.92	3- <i>O-p</i> -Coumaroylquinic acid	337.0941	337.0929	3.56	C ₁₆ H ₁₈ O ₈	phenolic acids	191.0553,163.0394,119.0499,93.0348
34	9.46	Caffeic acid methyl ester	193.0501	193.0506	-2.59	C ₁₀ H ₁₀ O ₄	others	174.0303,158.0332,129.0341,108.0210,89.0398
35	10.03	* <i>p</i> -Coumaric acid	163.0401	163.0401	0.12	C ₉ H ₈ O ₃	phenolic acids	119.0446,93.02906,65.03680,44.99623
36	10.16	4-Feruloylquinic acid	367.1047	367.1035	3.27	C ₁₇ H ₂₀ O ₉	phenolic acids	193.0496,173.0443,155.0360,134.0363,93.0342
37	10.95	5- <i>p</i> -Coumaroylquinic acid	337.0931	337.0929	0.59	C ₁₆ H ₁₈ O ₈	phenolic acids	191.0545,163.0392,127.0390,119.0484
38	11.16	Taxifolin	303.0525	303.0510	4.95	C ₁₅ H ₁₂ O ₇	flavonol and flavonol/flavone glycosides	285.0370,259.2642,241.0464,217.0521,125.0238,
39	11.34	*Ferulic acid	193.0509	193.0506	1.55	C ₁₀ H ₁₀ O ₄	others	178.0265,149.0368,134.0368
40	12.15	Suberic acid	173.0814	173.0819	-2.89	C ₈ H ₁₄ O ₄	others	130.9649,111.0809,83.0489
41	12.28	Myricetin-3- <i>O</i> -galactoside	479.0837	479.0831	1.25	C ₂₁ H ₂₀ O ₁₃	flavonol and flavonol/flavone glycosides	316.0220,287.0198,271.0242,259.0242,242.0207, 178.9970
42	12.48	Quercetagitrin	479.0816	479.0831	-3.13	C ₂₁ H ₂₀ O ₁₃	flavonol and flavonol/flavone glycosides	316.0219,287.0189,271.0243,259.0244,242.0211, 178.9980,151.0027
43	13.68	Myricetin-3- <i>O</i> -rhamnoside	463.0890	463.0882	1.73	C ₂₁ H ₂₀ O ₁₂	flavonol and flavonol/flavone glycosides	316.0236,287.0186,271.0254,101.0242
44	14.00	*Quercetin	301.0348	301.0354	-1.99	C ₁₅ H ₁₀ O ₇	flavonol and flavonol/flavone glycosides	271.0233,255.0278,227.0339,211.0388,151.0028, 121.0295,109.0295
45	14.30	*Quercetin-3- <i>O</i> -glucoside	463.0883	463.0882	0.22	C ₂₁ H ₂₀ O ₁₂	flavonol and flavonol/flavone glycosides	300.0273,271.0245,255.0296,243.0300
46	14.30	Quercetin 3- <i>O</i> -glucuronide	477.0681	477.0675	1.26	C ₂₁ H ₁₈ O ₁₃	flavonol and flavonol/flavone glycosides	301.0350,283.0245,255.0295,178.9982,151.0034, 121.0295
47	14.63	Quercetin-3- <i>O</i> -galactoside	463.0890	463.0882	1.73	C ₂₁ H ₂₀ O ₁₂	flavonol and flavonol/flavone glycosides	300.0271,271.0244,255.0293,243.0293,151.0027
48	15.74	Luteolin-7- <i>O</i> -glucuronide	461.0730	461.0725	1.08	C ₂₁ H ₁₈ O ₁₂	flavonol and flavonol/flavone glycosides	285.0397,257.0454,229.0499,85.0295,59.0139
49	16.01	Avicularin	433.0789	433.0776	3.00	C ₂₀ H ₁₈ O ₁₁	flavonol and flavonol/flavone glycosides	300.0243,271.0224,255.0247,151.0018,
50	16.04	Kaempferol-3- <i>O</i> -galactoside	447.0926	447.0933	-1.57	C ₂₁ H ₂₀ O ₁₁	flavonol and flavonol/flavone glycosides	284.0322,255.0294,227.0342,107.0131
51	16.15	Myricetin	317.0316	317.0303	4.10	C ₁₅ H ₁₀ O ₈	flavonol and flavonol/flavone glycosides	178.9985,151.0046,137.0242,109.0285,83.0124
52	16.20	*3,4-Dicaffeoylquinic Acid	515.1193	515.1195	-0.39	C ₂₅ H ₂₄ O ₁₂	phenolic acids	191.0563,179.0351,173.0458,161.0245,135.0451, 93.0350
53	16.60	Kaempferol-3- <i>O</i> -glucuronoside	461.0731	461.0725	1.30	C ₂₁ H ₁₈ O ₁₂	flavonol and flavonol/flavone glycosides	285.0404,257.0457,229.0512,213.0552,85.0299

54	16.60	*Kaempferol	285.0395	285.0405	-3.51	C ₁₅ H ₁₀ O ₆	flavonol and flavonol/flavone glycosides	255.0291,227.0349,187.0397,159.0436,143.0497, 117.0339,93.0344
55	16.83	*Quercitrin	447.0924	447.0933	-2.01	C ₂₁ H ₂₀ O ₁₁	flavonol and flavonol/flavone glycosides	300.0273,271.0247,255.0297,178.9983,151.0033, 121.0291
56	17.11	*Kaempferol-3- <i>O</i> -glucoside	447.0936	447.0933	0.67	C ₂₁ H ₂₀ O ₁₁	flavonol and flavonol/flavone glycosides	284.0324,255.0297,227.0347
57	17.13	Eriodictyol	287.0558	287.0561	-1.05	C ₁₅ H ₁₂ O ₆	flavonol and flavonol/flavone glycosides	151.0026,135.0448,107.0140,83.0139,65.0046
58	20.10	Kaempferol-3-rhamnoside	431.0973	431.0984	-2.55	C ₂₁ H ₂₀ O ₁₀	flavonol and flavonol/flavone glycosides	284.0317,255.0295,227.0344
59	21.19	*Naringenin	271.0603	271.0612	-3.32	C ₁₅ H ₁₂ O ₅	flavonol and flavonol/flavone glycosides	227.0355,151.0029,119.0492
60	21.22	Hieracin	301.0354	301.0354	0.00	C ₁₅ H ₁₀ O ₇	flavonol and flavonol/flavone glycosides	273.0375,227.0355,178.9985,151.0033,121.0295, 107.0138,83.0144
61	21.81	4-Oxododecanedioic acid	243.1232	243.1238	-2.47	C ₁₂ H ₂₀ O ₅	others	225.1132,207.1023,199.1337,181.1230,163.1132
62	23.86	Phloretin	273.0774	273.0768	2.20	C ₁₅ H ₁₄ O ₅	Ketones	167.0353,123.0467,107.0503,87.0096
63	25.03	Luteolin	285.0406	285.0405	0.35	C ₁₅ H ₁₀ O ₆	flavonol and flavonol/flavone glycosides	255.0291,227.0340,159.0439,117.0347,93.0350
64	25.28	Kaempferol-3-(2"-acetylramnoside)	473.1101	473.1089	2.54	C ₂₃ H ₂₂ O ₁₁	flavonol and flavonol/flavone glycosides	284.0316,255.0291,227.0340
65	26.78	Traumatic Acid	227.1297	227.1289	3.52	C ₁₂ H ₂₀ O ₄	others	209.1201,183.1411,165.1305
66	26.91	Trihydroxyoctadecadienoic acid	327.2186	327.2177	2.75	C ₁₈ H ₃₂ O ₅	others	291.1943,229.1430,211.1329,171.1015,85.0297
67	27.08	Kaempferol-3-(6"- <i>Z</i>)-Cinnamylglucoside)	577.1357	577.1351	1.04	C ₃₀ H ₂₆ O ₁₂	flavonol and flavonol/flavone glycosides	285.0383,255.0295,227.0339,145.0285,119.0496
68	32.86	Cyclocaric acid B	485.3265	485.3273	-1.55	C ₃₀ H ₄₆ O ₅	Terpenes	455.3126,439.3240,391.2993
69	54.46	Ursolic acid	455.3526	455.3531	-1.10	C ₃₀ H ₄₈ O ₃	others	407.3222
70	55.47	Hederagenin-3- <i>O</i> -arabinoside	603.3912	603.3902	1.66	C ₃₅ H ₅₆ O ₈	Terpenes	522.3130,472.3490,390.2714,372.2614,81.0710

317 **a:** Retention time (min); **b:** Precursor ion (m/z); **c:** Theoretical ion (m/z); *: Compound confirmed with reference standards