

Supplemental Materials

Liquid chromatography coupled with linear ion trap hybridOrbitrap mass spectrometry method for determination of alkaloids in the *Sinomeniumacutum*

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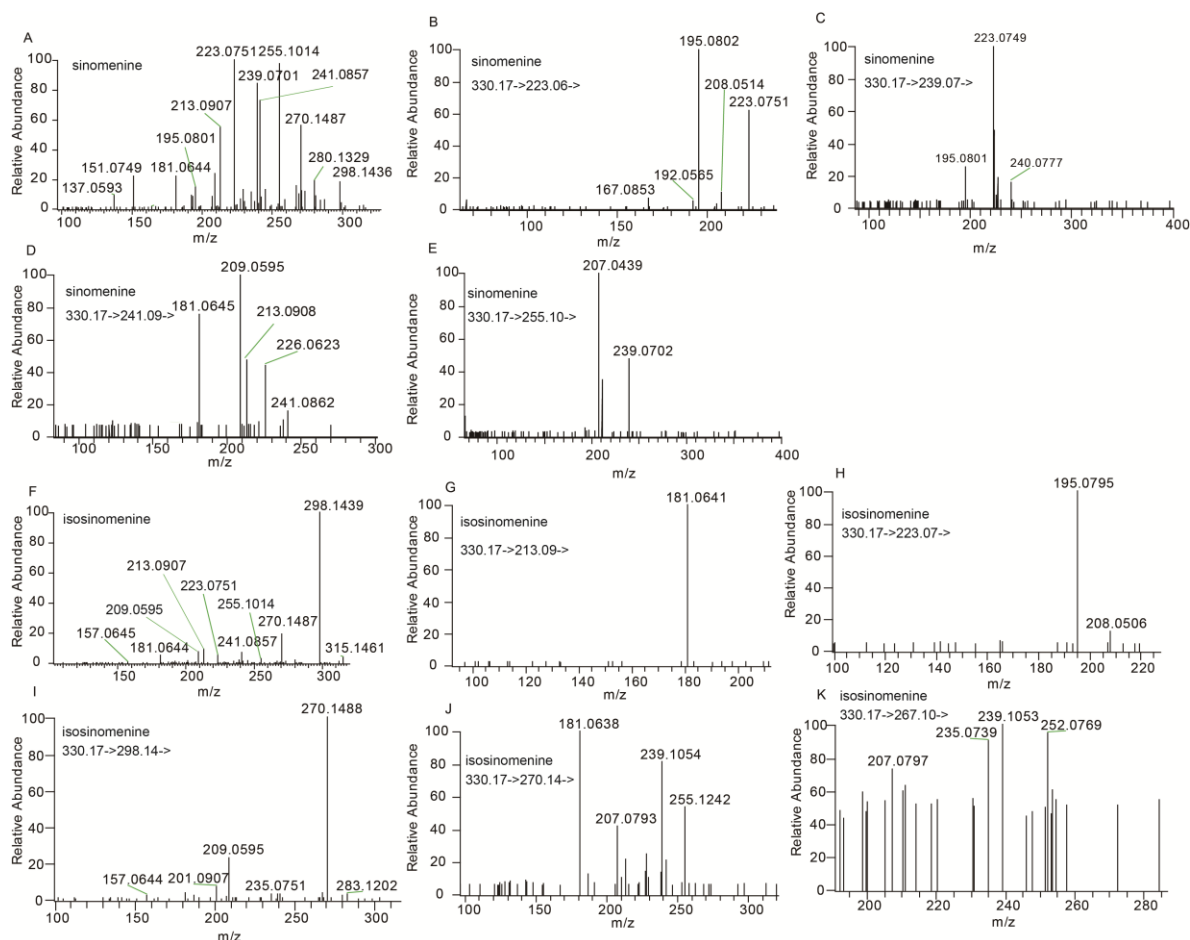


Figure S1. The MSⁿ spectra of the (A-E) sinomenine and (F-K) isosinomenine.

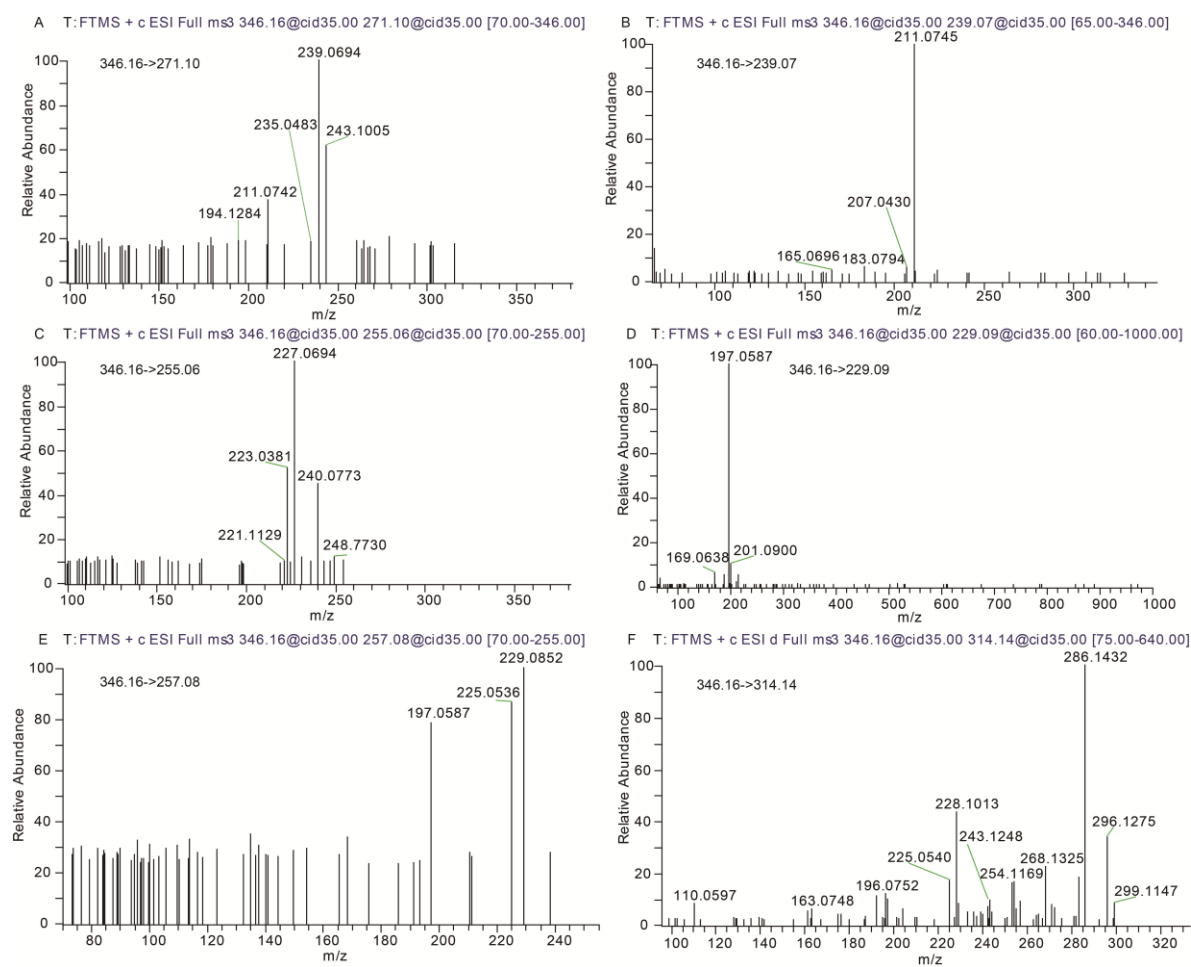


Figure S2. The MSⁿ spectra of the sinomenine N-oxide.

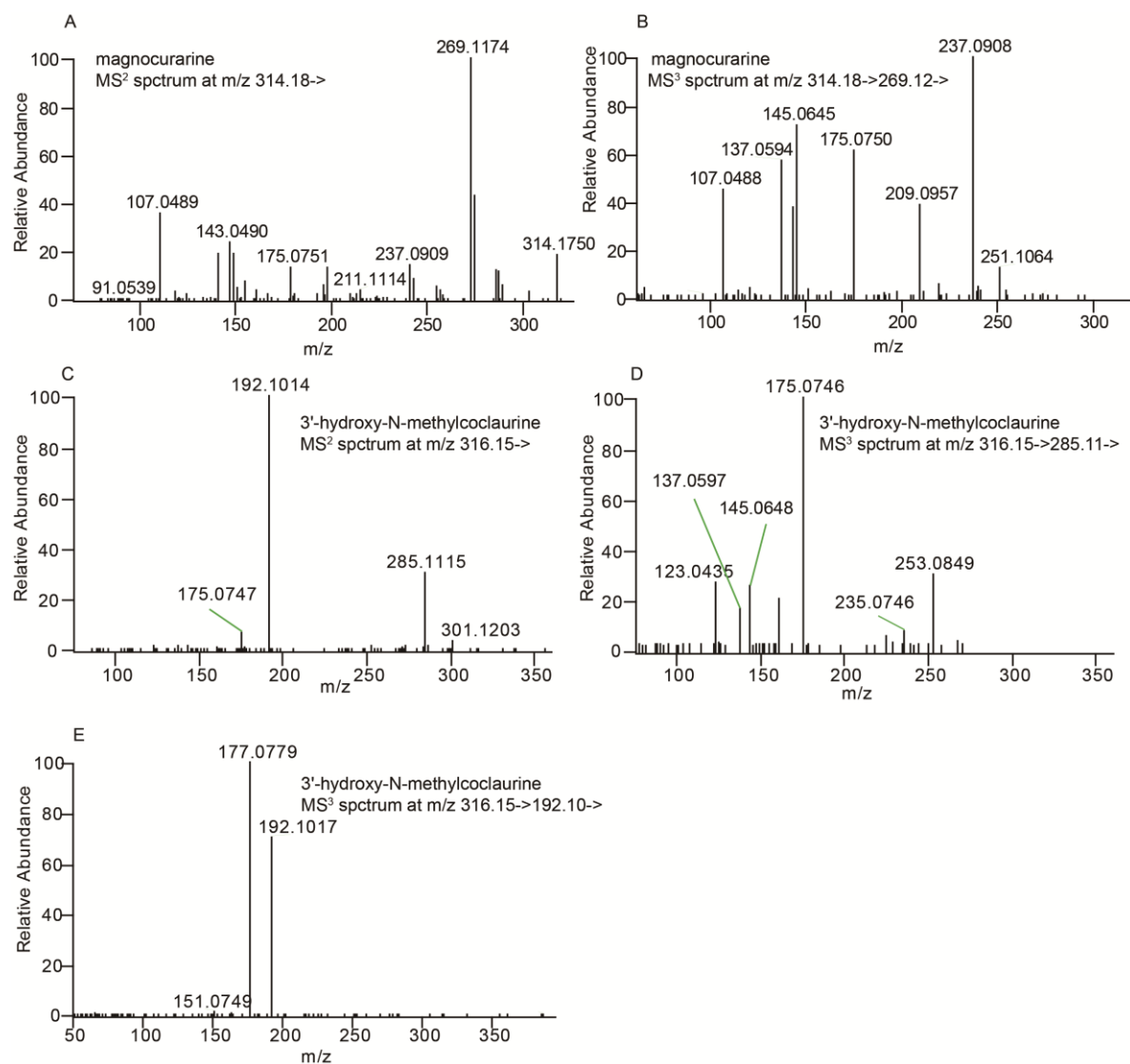


Figure S3. The comparison between the magnocurarine and 3'-hydroxy-N-methylcoclaurine, (A-B) the MSⁿ spectra of the magnocurarine, and (C-E) 3'-hydroxy-N-methyl coclaurine.

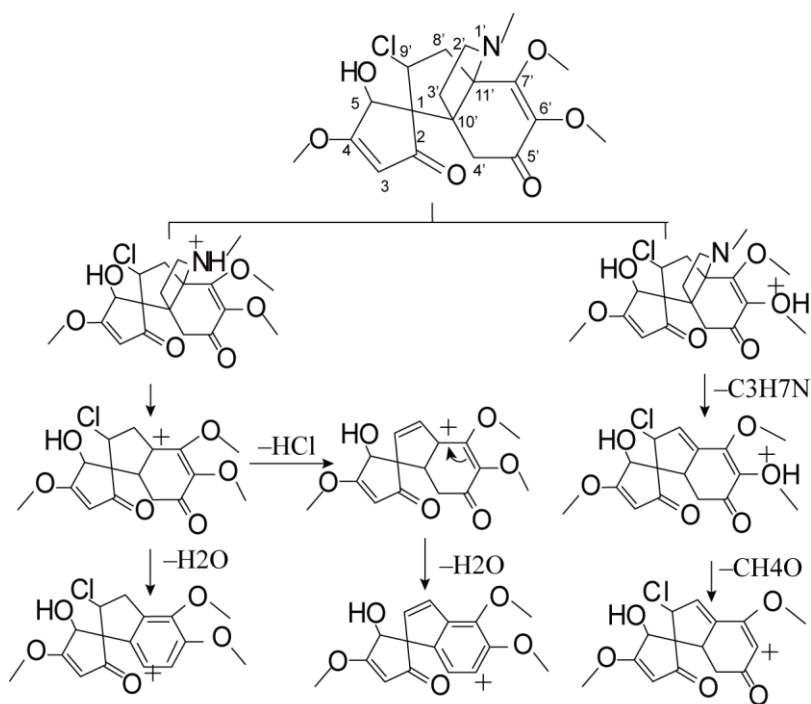


Figure S4. The proposed MS fragmentation pattern of the acutumine.

Table S1. MSⁿ data in positive mode of compound observed in the *Sinomeniumacutum*.

No	MS ² data	MS ³ data
1	223.0751, 241.0858, 255.1015, 267.1015, 273.1121, 287.1278 , 299.1278, 330.1699, 417.1545, 435.1650, 449.1807, 460.1966	223.0750, 255.1014
2	137.0591, 151.0747, 178.0856, 181.0644, 190.0855, 194.1168, 195.1015, 195.0801, 197.0589, 209.0594, 211.0746, 213.0902, 223.0751, 225.0539, 229.0851, 239.0695, 241.0855, 243.1246, 244.1324, 253.1012, 255.0644, 257.0800, 268.1324, 271.0956, 286.1429, 289.1066, 296.1272, 314.1377, 328.1532	[229.0851] 197.0589; [239.0695] 183.0796, 207.0432, 211.0745; [255.0644] 223.0385, 227.0694, 240.0772; [257.0800] 197.0590, 225.0539; [271.0956] 211.0744, 239.0695, 243.1005; [314.1383] 178.0857, 268.1326, 286.1431, 296.1274;
3	255.1014, 272.1282	107.0487, 123.0437, 136.0753, 143.0488, 145.0644, 161.0592, 255.1010
4	243.1014, 271.0964, 285.1122 , 303.1227, 317.1381, 447.1648, 465.1752, 479.1908, 490.2066, 504.2224	254.0935, 270.0884
5	257.0803, 328.1541	191.0696, 239.0699, 268.1328, 286.1432, 296.1277
6	137.0594, 157.0644, 183.0800, 193.0644, 201.0905, 211.0749, 215.1062, 243.1010 , 269.1166, 300.1587	137.0595, 155.0851, 161.0593, 183.0800, 193.0643, 201.0905, 211.0749, 215.1061, 228.0776
7	107.0488, 123.0438, 161.0894, 255.1010	107.0489, 123.0438, 145.0645, 161.0595
8	299.0915, 305.1205, 309.0525, 316.1180, 341.0780 , 348.1442, 352.0944, 367.0941	255.0652, 273.0757, 287.0916, 305.1021, 323.0682
9	181.0644, 193.0644, 195.0800, 209.0594, 213.0907, 223.0751, 239.0701, 241.0855, 255.1014 , 267.1012, 271.0963, 273.1117, 281.1168, 299.1273, 326.1382	195.0799, 223.0751, 227.1060, 240.0774
10	137.0595, 151.0752, 178.0859, 209.0594, 213.0907, 223.0750, 227.0701, 239.0699 , 241.0854, 255.1012, 256.1328, 259.0960, 267.1011, 269.1170, 271.0960, 273.1118, 287.1273, 299.1273	193.0643, 207.0436, 211.0748
11	137.0594, 165.0694, 181.0644, 183.0801, 187.0751, 193.0645, 195.0801, 201.0907, 211.0751, 213.0907 , 215.1062, 225.0906, 227.1065, 229.1095, 243.1012, 251.1063, 257.1168, 269.1171, 275.1279, 283.1329, 300.1593, 314.1750	153.0694, 181.0644, 185.0957, 198.0671
12	269.1174, 286.1438	107.0487, 151.0750, 175.075, 269.1172
13	77.0781, 192.1020 , 316.1540	151.0749, 177.0779
14	137.0594, 151.0749, 181.0643, 192.1017, 193.1095, 195.0802, 207.0802, 209.0593, 213.0906, 223.0751, 239.0700, 241.0856, 255.1013, 259.0964, 267.1013, 270.1486, 271.0963, 273.1120, 280.1326, 287.1277, 298.1436	[223.0751]195.0802, 208.0514, 223.0750; [239.0700]207.0439, 211.0753, 239.0702; [241.0856]181.0645, 209.0594, 213.0908, 226.0623; [255.1013] 195.0801, 223.0749, 227.1059, 240.0780; [270.1486]195.0800, 227.1063, 255.1252
15	305.1021, 341.0786 , 362.1597, 366.1100	287.0915, 305.1021, 323.0681
16	175.0748, 192.1017, 285.1118	[192.1017]177.0779, 192.1016; [285.1118]115.0536, 123.0434, 137.0590, 143.0485,

		161.05906, 175.0745, 253.0850
17	137.0594, 151.075, 299.1155 , 314.1385	252.1017, 280.0972, 283.0839
18	269.1172 , 314.1749	107.0487, 269.1169, 299.1513
19	225.0907, 253.0857, 281.0808, 313.1070	225.0905, 253.0857, 281.0808, 298.0834
20	137.0595, 151.0751, 167.0336, 192.1014, 211.0385, 243.0648, 257.0804, 258.1123, 269.0808, 271.0600, 275.0910, 285.1116, 297.0756, 300.1226, 303.1221, 311.0908, 317.1377, 328.1178, 332.1485, 342.1328, 345.1202	[275.0910] 211.0385, 243.0651, 247.0958, 257.0803; [328.1178] 272.1272, 296.1274, 300.1222
21	253.0857, 285.1121, 295.0963, 313.1071 , 328.1540, 340.1540	223.0594, 253.0858, 281.0808, 285.0756
22	107.0488, 137.0594, 145.0644, 151.0750, 163.0750, 175.0750, 178.0858, 269.1174 , 286.1437, 450.1633, 495.2211, 509.1597, 511.1752, 514.2222, 517.2333, 526.2223, 540.2380, 557.2647,	107.0488, 137.0594, 143.0489, 145.0645, 175.0749, 209.9573, 237.0908
23	566.2174, 568.2332, 582.2490, 584.2282, 586.2433, 597.2966, 598.2440, 600.2590 , 614.2745, 625.2904, 639.2698, 642.2931	387.1223, 433.1428, 451.1534, 461.1375, 479.1481, 483.1795, 493.1635, 511.1742, 525.1898, 540.2369, 558.2473, 568.2318, 582.2478, 585.2345
24	243.1014, 271.0964, 285.1122 , 303.1228, 317.1382, 329.1382	254.0936, 270.0885
25	107.0488, 137.0594, 143.0489, 145.0645, 151.0750, 175.075, 192.1015, 237.0909, 269.1173	107.0488, 137.0594, 145.0645, 175.0750, 237.0908
26	161.0833, 192.1018, 254.0937, 269.1173, 281.1174	[192.1018] 161.0832, 177.0881; [269.1173] 209.0951, 237.0900, 238.0979, 241.0849, 254.0927; [281.1174] 249.0901, 250.0979, 253.1214, 266.0928
27	285.1123, 295.0966, 313.1073 , 340.1542	223.0594, 253.0857, 281.0808, 285.0757
28	137.0594, 143.0488, 151.0750, 175.0750, 235.0751, 267.1015, 299.1280 , 301.1434, 345.1886	137.0593, 151.0751, 175.0749, 235.0750, 267.1013
29	151.0749, 178.0858 , 265.0857, 283.1328, 297.1120, 313.1306	118.0648, 146.0596, 163.0624
30	293.0807, 325.1069 , 339.1223	237.0910, 265.0858, 282.0886, 293.0809, 297.1121, 307.0966, 310.0834
31	265.0857, 279.1014, 297.1122 , 311.1273	237.09067, 265.08597, 282.0884
32	296.1283, 298.1075, 313.1311	280.09671, 298.1075
33	137.0593, 151.0750, 157.0645, 181.0644, 187.0748, 190.0858, 192.1014, 201.0907, 209.0595, 213.0907, 223.0751, 239.0701, 241.0857, 245.1170, 255.1014, 267.1015, 270.1487, 273.1118, 280.1330, 298.1439, 315.1461	[209.0595] 181.0638; [213.0907] 181.0638; [223.0752] 195.0794, 208.0505; [241.0857] 153.0326, 165.0252, 181.0666, 209.0592, 213.0907; [267.1015] 235.0739; [270.1487] 181.0638, 239.1054, 255.1242; [298.1439] 157.0644, 181.0647, 187.0749, 201.0907, 209.0595
34	151.0747, 192.1015, 207.0742, 211.0751, 233.0586, 237.0908, 239.0701, 243.1011, 253.0856, 265.0859, 268.1332, 271.0963, 282.1121, 285.1182, 296.1279, 297.1121, 313.1307	[239.0701] 207.0431, 211.0743; [265.0859] 233.0594, 237.0906; [285.1182] 197.0952, 221.0588, 225.0901, 242.0928, 253.0850, 257.1164, 270.0873
35	300.0630, 315.0865	223.0388, 255.0651, 300.0628
36	263.0703, 295.0971 , 308.1281	245.0596, 263.0701, 277.0857
37	107.0488, 137.0595, 143.0489, 145.0645, 151.0750, 157.0645, 175.0749, 194.1173, 237.0908, 239.1064, 269.0908 , 271.1328	107.0486, 137.0594, 145.0643, 175.0749, 209.0957, 237.0906, 251.1064
38	265.0859, 297.1124	233.0594, 237.0907, 265.0859, 282.0883
39	279.1072, 293.0117, 299.1272, 311.1276 , 325.1429	248.0830, 279.1016, 296.1040

40	269.0808, 330.0735, 345.0965	269.0808, 285.0757, 295.0601, 299.0930
41	336.1229, 353.1256	336.1227
42	279.0889, 294.1124, 307.0841	251.0384, 279.0889
43	280.0969, 309.0999 , 324.1227	281.1046, 294.0763
44	279.0889, 294.1124, 307.0841	251.0384, 279.0889
45	280.1094, 296.1043, 311.1280	280.1095, 296.1042
46	329.1018	255.0649, 314.078
47	294.1123, 322.1076, 323.1151	279.0890, 295.1205, 308.0919
48	294.1123, 322.1076, 323.1151	279.0890, 295.1205, 308.0919
49	294.1123, 322.1076, 323.1151	279.0890, 295.1205, 308.0919
50	292.0969, 308.1283, 320.0920 , 321.0996	290.0813, 282.0968, 318.0759
51	294.1123, 322.1076, 323.1151	279.0890, 295.1205, 308.0919
52	308.1279, 336.1231, 337.1306	308.1279, 320.0916, 321.0992, 334.1072

Italic and bold in the MS² data represented the parent ion for the MS³ data by Orbitrap MS.

Italic and bold in box in the MS³ data represented the parent ion for the MS³ data by Orbitrap, and followed was the MS³ information

Table S2. MSⁿ information of the standards.

t _R (min)	Compounds ¹	m/z	[M+H] ⁺	ppm	MS ² information	MS ³ information
16.66	Tetrahydroberberine	340.1539	C ₂₀ H ₂₂ O ₄ N	-0.405	150.0672, 165.0906, 192.1015	148.0752, 177.0778, 192.1012
17.88	Tetrahydropalmatine	356.1854	C ₂₁ H ₂₆ O ₄ N	-0.245	150.0673, 165.0907, 192.1019	148.0752, 176.0702, 177.0779, 192.1014
19.62	Berberrubine	322.1072	C ₁₉ H ₁₆ O ₄ N	-0.204	307.0832	279.0888, 307.0834
21.13	Berberine	336.1227	C ₂₀ H ₁₈ O ₄ N	-0.295	292.0966, 320.0921, 321.0993	290.0817, 292.0966, 318.0755

¹These standards were not detected in the *Sinomeniumacutum*, others who detected in the study were illustrated in the Table 1.