

2) ニンジン

得られた ESI ポジティブモード及びネガティブモードそれぞれのクロマトグラム (図 17,18) を比較すると、絶対強度ではネガティブモードのスケールはポジティブモードの 3 倍あり、主なニンジンサポニン類と思われるピークはネガティブモードでより高感度で検出されることが判明した。また、ポジティブモードでは MS/MS においてフラグメンテーションを観測出来なかった。

ギンセノシド Rg1 の標品の保持時間 12.8 分付近に検出されたピーク 1 はマススペクトル (図 19) から、ギンセノシド Rg1 のほかにギンセノシド Re の共溶出が認められた。ギンセノシド Rg1 の酢酸付加イオンピーク m/z 859 及び $[M-H]^-$ イオンピーク m/z 799 をプリカーサーイオンとした MS/MS (図 20 及び図 21) では、前者の酢酸付加イオンピークでは、 m/z 799 ($[M-H]^-$) を主とし、さらにグルコースの脱離した m/z 673 が観測された。後者の $[M-H]^-$ イオンピークの場合は、グルコースの解離した m/z 673 を主とし、さらにグルコースの解離した m/z 475 や脱水した m/z 619 が観測された。一方、ギンセノシド Re の $[M-H]^-$ イオンピーク m/z 945 をプリカーサーイオンとした MS/MS (図 22) では、グルコースの解離した m/z 783 を主とし、さらにラムノースの解離した m/z 637 やこれらの脱水ピーク m/z 765 及び m/z 619、また m/z 637 からさらにグルコースの解離した m/z 475 及び $[M-H]^-$ m/z 945 からラムノースの解離した m/z 799 が観測された。

ギンセノシド Rb1 の標品の保持時間

18.1 分付近に検出されたピーク 2 はマススペクトル (図 23) の比較からギンセノシド Rb1 と同定された。 m/z 1107 ($[M-H]^-$) を主とし、さらに 2 価イオン m/z 553 が観測された。2 価イオン m/z 553 をプリカーサーイオンとした MS/MS (図 24) では、グルコースの解離した m/z 945 を主とし、さらにグルコースの解離した m/z 783 が観測された。

これらニンジンサポニン類 3 成分のスペクトル解析の結果から、本分析条件によってニンジンに特徴的に含まれる成分についての化学情報の集積が可能であると考えられた。

E. 結論

繁用漢方処方薬であるカンゾウについて、LC-MS/MS を用いた分析プロファイルから、生薬の化学成分情報のデータベース化を行い、品質の情報化を試みることにした。そこで、HPLC の移動相の種類やグラジエント条件の検討、MS 条件や MS/MS 条件の検討及び分析時間の検討等を行い、データ採取条件の検討を行った。その結果、カンゾウ及びニンジンに含まれる成分についての化学情報の集積が可能となった。

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F. 研究発表

1. 論文発表

なし

2. 学会発表等

なし

G. 知的財産権の出願・登録状況

なし

表1 LC-MS/MS測定により得られたカンゾウの成分情報(1)

No	極性	推定組成	保持時間	プリカーサ質量(強度)	プロダクト質量(相対強度)
1	Pos		3.55	336.0662(8.0E6)	313.0500(40), 295.0395(100: 2.59E6), 277.0288(3), 251.0494(1), 200.9973(1.5)
2	Pos	C28H13O6		445.0706 (5.60E6)	427.0602(12), 401.0810(3), 383.0705(7), 351.0190(50), 339.0290(100: 1.79E6), 321.0184(3), 253.0283(45), 232.9867(20)
	Neg	C28H11O6	5.79	443.0554 (5.12E5)	293.0866 (100: 9.18E3), 233.0658 (35)
3	Neg			472.0089 (5.49E5)	428.0181(100: 1.43E5), 384.0265(20), 340.0388(30), 321.9768(25), 219.9821(40)
4	Pos	C21H23O9	6.9	419.1336 (4.96E6)	257.0806 (100: 4.19E6)
				257.0813 (C15H13O4)	239.0703(40), 214.9875(100: 5.42E5), 147.0438(60), 137.0230(55)
5	Pos	C27H33O14, 418+Glu		581.1853 (6.02E5)	
		581+NH3		598.2118	581.1868(2), 419.1337(100: 1.19E6), 257.0807(70)
6	Pos	C18H25O12	6.94	433.1339 (5.42E6)	415.1244(5), 397.1140(4), 307.1031(12), 289.0923(10), 271.0818(8), 187.0601(2), 163.0599(4), 145.0493(10), 127.0387(100: 7.13E5)
7	Pos	C27H31O15, 580+O-2H	7.7	595.1643 (4.67E6)	577.1570(100: 2.03E6), 559.1463(30), 541.1356(10), 529.1356(20), 523.1250(20), 511.1250(30), 499.1248(20), 481.1143(10), 457.1141(100: 8.52E5)
8	Neg	C15H11O4, 418-Glu	7.72	255.0653 (1.82E6)	135.0087(100: 1.44E5)
9	Neg	C27H31O14, 418+Glu		579.1712(1.58E6)	417.1172(100: 1.02E6)
				417.1181 (C21H21O9)	297.0760(2), 135.0087(14)
10	Neg	C18H23O12	7.8	431.1185 (1.87E6)	387.1278(4), 369.1174(40), 329.0864(100: 1.89E5), 305.0865(7), 287.0761(8), 269.0445(6), 243.0865(15), 225.0760(5), 203.0555(20), 191.0345(2), 179.0346(5), 161.0453(3), 125.0246(2)
				711.2141 (1.93E6)	549.1584(100: 1.73E6)
11	Neg	C32H39O18, 550+Glu	7.93	549.1607 (C26H29O13)	429.1172(50), 417.1175(95), 399.1070(20), 357.0968(10), 327.0862(5), 297.0759(100: 2.37E4), 256.0685(80)
				565.1542 (8.20E6)	547.1459(100: 3.47E6), 529.1353(30), 511.1246(20), 499.1245(25), 481.1139(10), 469.1139(10), 457.1138(10), 445.1139(10), 427.1033(15)
12	Pos	C26H29O14, 418-2H+Xly+O	8.83	565.1542 (8.20E6)	547.1459(100: 3.47E6), 529.1353(30), 511.1246(20), 499.1245(25), 481.1139(10), 469.1139(10), 457.1138(10), 445.1139(10), 427.1033(15)
				563.1399 (8.06E6)	545.1270(30), 503.1168(65), 473.1066(100: 1.18E5), 443.0963(60), 425.0858(15), 383.0755(40), 353.0650(50)
13	Pos	C27H33O14, 418+Glu	9.24	581.1853 (4.33E6)	419.1337(2), 257.0806(100: 3.26E6)
				579.1712 (5.12E6)	579(100: 7.43E5), 489.1022(4), 256.0686(1)
14	Pos	C26H29O13, 418-2H+Xly	9.4	549.1591 (1.06E6)	417.1176(1), 255.0646(100: 1.42E6)
				547.1450 (7.89E5)	415.1018(30), 295.0602(6), 253.0499(100: 3.43E5)
15	Neg	C32H39O18, 550+Glu	9.42	711.2139 (1.84E6)	693.2000(4), 621.1793(2), 591.1533(10), 579.1685(60), 561.1581(15), 549.1584(100: 8.76E4), 531.1481(15), 429.1172(25), 297.0757(35), 256.0685(35)
16	Pos	C21H21O9	9.62	417.1179 (4.08E6)	255.0654(100: 4.83E6)
				415.1026 (3.74E5)	253.0498(100: 3.31E5)
17	Pos	C26H29O13, 418-2H+Xly	9.65	549.1589 (1.46E6)	
				547.1449 (6.94E5)	
18		C32H39O18, 550+Glu		711.2139 (8.92E5)	691.1826(2), 605.1473(5), 591.1682(10), 549.1582(80), 531.1479(100: 1.06E5), 417.1171(20), 399.1067(15), 297.0756(12), 256.0685(10)
19		C33H37O19, 712+CH2O		737.1931 (1.17E6)	719.1780(1), 675.1882(4), 635.1575(4), 593.1474(15), 575.1371(5), 557.1266(5), 503.1167(20), 473.1067(100: 6.89E5), 383.0753(10), 353.0650(15)
20	Neg	C21H19O9	9.83	415.1025 (1.34E6)	
				253.0495 (C15H9O4)	253(100: 1.67E4), 235.0389(15), 225.0548(30), 209.0600(35), 185.0602(25), 135.0086(30)
21	Pos	C27H31O14, 416+Glu	10	579.1692 (8.26E6)	561.1609(100: 3.47E6), 543.1503(55), 525.1396(30), 513.1396(20), 495.1290(10), 483.1289(10), 457.1133(20), 441.1184(10), 423.1078(5)
				577.1556 (7.07E6)	577(100: 9.71E5), 559.1425(15), 503.1166(30), 487.1219(25), 473.1064(30), 457.1117(60), 439.1014(6), 413.0858(10), 383.0754(40), 353.0652(35), 335.0548(2)
22	Pos	C21H23O9	10.18	419.1333 (6.83E6)	257.0811(100: 5.80E6)
				257.0812 (C15H13O4)	239.0704(70), 214.9875(50), 211.0753(30), 163.0387(15), 147.0438(95), 137.0230(100: 8.18E5)
23	Neg	C26H29O13, 418+Xly	10.32	549.1608 (2.30E6)	429.1022(100: 2.09E5), 417.1172(5), 387.1068(2), 309.0604(4), 297.0756(20), 256.0685(20), 219.0292(4)

表1 LC-MS/MS測定により得られたカンゾウの成分情報(2)

No	極性	推定組成	保持時間	プリカーサー質量(強度)	プロダクト質量(相対強度)
24	Neg	C27H31O14, 418+Glu		579.1712 (2.49E6)	579(100: 1.33E5), 559.1429(10), 503.1171(20), 487.1227(5), 473.1069(15), 457.1119(25), 417.1173(5), 383.0757(15), 353.0653(12), 323.0971(15), 283.0602(25), 256.0685(25)
25	Neg	C32H35O18, 550-4H+Glu		707.1831 (6.11E5)	689.1667(2), 645.1776(6), 605.1470(15), 563.1368(60), 545.1266(10), 527.1164(4), 473.1063(20), 443.0960(100: 1.59E5), 425.0856(2), 383.0753(10), 353.0650(15)
26	Neg	C32H39O18, 550+Glu		711.2140 (8.92E5)	691.1838(10), 647.1810(6), 579.1685(95), 565.1424(20), 549.1583(90), 531.1479(100: 2.28E4), 445.1021(40), 297.0757(20), 256.0685(30)
22	Neg	C21H21O9	10.39	417.1182 (1.75E6)	417(60), 399.1074(6), 297.0760(35), 255(100: 1.25E4), 253.0505(50)
				255.0653 (C15H11O4)	135.0084(100: 7.06E5), 119.0500(15)
27	Pos	C26H31O13, 418+Xly	10.43	551.1741 (9.80E6)	419.1346(6), 257.0811(100: 6.80E6)
28	Pos	C21H23O9		419.1331(9.54E6)	257.0804(100: 1.27E6)
				257.081 (C15H13O4)	239.0700(70), 211.0749(30), 163.0384(15), 147.0435(95), 137.0228(100: 1.81E7), 119.0486(5)
		(418*2+H)		837.2552	675.2059(15), 581.1853(10), 419.1331(5), 257.0806(100: 2.82E6)
29	Pos			969.2951 (9.87E6)	
27	Neg	C26H29O13, 418+Xly	10.54	549.1607 (7.34E7)	549(20), 531.1495(2), 429.1172(60), 417.1175(3.49E6), 399.1071(20), 387.1074(5), 357.0966(10), 327.0864(6), 297.0758(95), 269.0809(15), 256.0685(80)
30	Pos	C32H37O18	10.59	709.1949 (2.77E6)	619.1899(100: 6.35E5), 673.1793(70), 655.1685(70), 643.1685(20), 625.1680(15), 619.1680(20), 601.1573(10), 571.1464(20), 511.1245(5), 499.1248(10), 445.1140(15), 427.1035(80), 409.0927(25), 379.0822(5), 355.0822(5), 325.0715(5)
28	Neg	C21H21O9	10.64	417.1182 (6.59E7)	417(100: 2.75E6), 297.0759(4), 255(20), 135.0087(20)
31	Neg	C26H29O14, 418+Xly+O	12.11	565.1554 (3.69E6)	565(40), 521.1633(10), 497.1638(12), 479.1532(8), 433.1119(25), 415.1015(4), 389.1224(4), 313.0704(8), 271.0600(100: 5.24E5), 257.0809(2), 245.0809(4), 227.0704(35), 203.0706(10), 185.0602(5), 177.0189(5), 161.0605(3)
32	Pos	C24H25O12	12.21	505.1332 (1.48E6)	386.0767(6), 257.0806(100: 1.01E6)
33	Pos	C15H13O5, Licodione	12.3	273.0762 (6.07E6)	255.0650(20), 231.0647(5), 189.0542(3), 179.0334(5), 163.0385(20), 153.0177(100: 1.60E6), 147.0435(70), 137.0228(2.5), 119.0487(5)
	Neg	C15H11O5, Licodione	12.38	271.0602 (4.93E6)	271(15), 253.0496(8), 237.0547(13), 227.0705(10), 177.0190(60), 165.0191(8), 151.0035(100: 8.83E4), 135.0088(4)
34		C21H21O10		433.1131 (6.01E6)	313.0703(0.5), 271.0600(100: 4.51E6), 177.0188(0.5), 151.0034(1)
35	Pos	C26H31O13	13.19	551.1741 (2.16E7)	419.1341(70), 389.1234(4), 257.0808(100: 3.27E6)
	Neg	C26H29O13	13.21	549.1604 (3.15E7)	429.1169(15), 417.1170(40), 297.0756(40), 256.0685(100: 1.05E4)
36	Pos	C27H31O13	13.48	563.1749 (1.85E7)	431.1334(1), 269.0806(100: 5.57E6), 254.0571(1.5), 237.0542(1), 213.0905(0.8)
	Neg	C27H29O13	13.51	561.1606 (9.26E6)	561(40), 309.0755(15), 281.0807(2), 267.0652(100: 1.03E6), 252.0419(20)
37	Pos	C21H23O9	13.6	419.1337 (5.38E7)	257.0813(100: 1.53E7), 239.0706(0.3), 147.0437(0.3), 137.0231(0.2)
	Neg	C21H21O9	13.63	417.1180 (4.06E7)	417(40), 339.0865(4), 321.0759(5), 311.0917(6), 297.0761(100: 1.14E6), 269.0812(15), 256.0686(20), 135.0087(30)
38	Pos	C22H23O9	13.88	431.1336 (2.35E7)	269.0807(100: 1.01E7)
39	Neg	C24H23O11	13.94	489.1392 (2.47E6)	489(20), 429.2268(5), 267.0650(100: 1.53E6), 252.0418(2)
				267.0652 (C16H12O4)	267(30), 252.0423(100: 3.12E6)
40	Pos	C35H37O15	14.01	697.2104 (1.95E6)	697(15), 535.1597(10), 441.1388(5), 279.0862(27), 261.0755(100: 3.32E5), 243.0648(20), 215.0698(10)
41	Pos	C23H25O10	14.07	461.1437 (1.72E6)	299.0913(100: 2.07E6)
42	Pos	C54H85O24		1117.5341 (5.70E5)	
43	Pos	C16H15O5, Licochalcon B		287.0918 (1.62E6)	269.0812(5), 245.0810(98), 193.0495(15), 167.0337(19), 151.0387(100: 7.28E5), 121.0282(15)
44	Neg	C36H37O16, 550+GluUA	14.16	725.2084 (7.75E6)	725(20), 579.1673(4), 549.1579(100: 1.59E6), 531.1479(80), 417.1171(7), 399.1067(12), 297.0755(1), 256.0685(3)
	Pos	C36H39O16, 550+GluUA	14.17	727.2207 (3.63E6)	709.2153(20), 565.1720(10), 471.1509(8), 445.1135(5), 339.1084(5), 309.0973(50), 291.0868(100: 3.52E5), 273.0760(10), 245.0809(15), 227.0702(4)
42	Neg	C54H83O24	14.22	1115.5258 (2.34E6)	
45	Pos	C15H13O4, 418-Glu	14.35	257.0813 (4.11E7)	242.0568(30), 239.0698(80), 211.0747(35), 163.0382(15), 147.0433(95), 137.0226(100: 2.54E6), 119.0485(5)
	Neg	C15H11O4, 418-Glu	14.39	255.0654 (1.13E7)	255(10), 211.0755(1), 153.0191(4), 135.0085(100: 1.88E6), 119.0503(10)

表1 LC-MS/MS測定により得られたカンゾウの成分情報(3)

No	極性	推定組成	保持時間	プリカーサ質量(強度)	プロダクト質量(相対強度)
46	Pos	C42H63O17, 822+O	15.34	839.4032 (3.75E6)	821.3944(1.5), 803.3845(2), 785.3738(2.5), 663.3729(2), 645.3624(20), 627.3519(60), 609.3414(35), 591.3301(1.5), 563.3362(2), 487.3414(2.5), 469.3307(100: 7.19E5), 451.3203(80), 439.3204(5), 433.3097(25), 421.3098(4), 405.3152(8), 393.2786(6)
	Neg	C42H61O17, 822+O	15.54	837.3896 (8.84E6)	837(35), 819.3768(12), 793.3978(3), 775.3875(7), 703.3663(1), 661.3564(13), 485.3256(1), 351.0556(100: 1.40E6), 333.0450(2), 289.0554(2.5)
47	Neg	C36H37O16, 550+GluUA	15.7	725.2067 (3.86E6)	725(50), 549.1578(40), 531.1480(100: 1.29E6), 417.1172(2), 399.1067(5), 297.0757(1), 256.0686(1)
	Pos	C36H39O16, 550+GluUA	15.72	727.2207 (2.29E6)	709.2129(7), 617.1860(5), 565.1708(50), 547.1602(8), 461.1444(7), 419.1335(10), 309.0966(30), 291.0860(90), 257.0804(100: 1.09E5)
48	Neg	C21H21O7, Glycycooumarin+2O+2H	15.82	385.1282 (1.56E6)	370.1040(15), 341.1379(4), 311.0547(100: 7.00E5), 297.0393(20), 284.0315(1.5), 267.0652(2), 221.0811(2)
49	Pos	C42H65O16	16.17	825.4245(7.78E6)	649.3956(30), 473.3634(5), 455.3528(100: 8.57E5), 437.3422(2), 419.3315(2)
	Neg	C42H63O16	16.32	823.4091 (2.17E7)	823(25), 805.3980(10), 761.4087(5), 647.3774(10), 351.0555(100: 3.40E6), 289.0554(4)
50	Pos	C30H45O3	16.49	453.3359 (1.88E6)	435.3257(100: 6.14E5)
51	Pos	C42H61O17, 822+O-2H		837.3863 (2.15E6)	
52	Pos	C48H73O22, 822+O+Glu	16.55	1001.4569 (5.63E6)	983.4503(5), 825.4288(80), 807.4182(5), 663.3754(10), 649.3962(80), 631.3857(50), 487.3430(100: 1.13E6), 469.3325(80), 451.3221(10)
53	Pos	C18H15O4, 256+CH2	16.64	271.0969 (5.03E6)	229.0861(100: 4.23E6), 177.0545(5), 151.0387(4), 121.0281(7)
54	Pos	C21H21O7, Glycycooumarin+2O		385.1283 (5.60E6)	367.1184(20), 357.1342(3), 339.0870(5), 335.0921(6), 313.0714(100: 2.92E6), 301.0713(10), 285.0763(20), 203.0339(2), 149.0231(3)
53	Neg	C18H13O4, 256+CH2	16.65	269.0809 (1.59E6)	
54	Neg	C21H19O7, Glycycooumarin+2O		383.1122 (3.20E6)	383(20), 368.0885(100: 1.64E6), 338.0781(10), 323.0546(10), 311.0547(30), 269.0315(7), 285.0393(8)
55	Neg	C42H61O16		821.3937 (1.00E7)	803.3826(20), 777.4034(3), 759.3927(10), 645.3620(15), 627.3514(3), 351.0555(100: 1.20E6), 333.0449(2), 289.0554(5)
56	Neg	C48H69O21, 822-2H+Glu		981.4294 (1.70E6)	981(30), 963.4193(10), 919.4290(5), 659.3413(10), 497.1133(100: 3.33E5), 479.1025(2), 453.1234(3), 435.1130(20), 407.1180(4), 399.0920(17), 321.0815(18)
57	Neg	837.3886(1価イオンに交換), C42H61O17	16.75	418.1904 (2-, 3.88E6)	661.3564(5), 643.3462(8), 567.3309(1), 485.3255(100: 1.71E6), 419.1935(5), 499.1852(10), 387.1903(5), 351.0555(30), 330.1747(10), 289.0554(3), 193.0346(7), 175.0242(2)
58	Neg	999.4408(1価イオンに交換), C48H71O22		499.2165 (2-, 7.18E6)	879.3983(4), 837.3879(3), 499.7184(1), 418.1910(100: 3.52E6)
59	Neg	C42H59O17, 822+O-2H		835.3720 (9.47E6)	835(20), 817.3619(10), 773.3719(5), 659.3412(15), 351.0555(100: 1.25E6), 289.0554(5)
58	Neg	C48H71O22, 822+O+Glu		999.4395 (7.17E6)	879.3979(4), 837.3879(100: 1.2E6), 819.3781(20), 775.3885(1), 661.3568(10), 643.3467(1), 351.0556(15)
60	Pos	C44H65O19, 881+16	17.12	897.4081 (1.57E7)	861.3922(2), 721.3808(10), 703.3705(20), 685.3599(30), 545.3484(100: 3.26E6), 527.3379(90), 509.3275(15), 467.3168(2)
61	Pos	C42H63O16	17.25	823.4076 (5.23E6)	805.3996(15), 787.3889(5), 647.3784(25), 629.3683(2), 471.3467(3), 453.3360(100: 9.15E5), 435.3256(4)
62	Neg	C44H63O19, 879+16	17.37	895.3929 (3.20E7)	895(25), 877.3823(12), 833.3926(8), 791.3823(1), 773.3721(2), 719.3619(12), 659.3411(7), 641.3302(2), 351.0555(100: 2.25E6), 333.0450(2), 289.0554(3)
61	Neg	C42H61O16	17.44	821.3935 (2.32E7)	803.3827(13), 759.3930(10), 687.3716(2), 645.3620(12), 627.3512(3), 351.0555(100: 5.76E5), 333.0452(2), 289.0553(3)
63	Pos	C48H73O21, 822+Glu	17.43	985.4614 (2.86E7)	823.4141(1), 809.4337(20), 647.3805(10), 633.4012(8), 615.3906(50), 471.3480(25), 453.3375(100: 2.47E6), 435.3270(3), 407.3323(3), 389.3215(1)
65	Neg	821.3938(1価イオンに交換), C42H61O16	17.62	410.1930 (2-, 2.56E7)	645.3618(3), 627.3514(5), 537.3565(2), 497.3253(1), 469.3307(100: 1.78E6), 411.1962(20), 401.1879(3), 379.1930(10), 351.0557(35), 322.1773(5), 289.0554(5), 193.0346(7), 175.0241(3)
	Neg	984の2価イオン		491.2193 (2-, 1.80E7)	863.4034(3), 821.3931(2), 803.3829(1), 431.1981(1), 410.1934(100: 7.50E6), 401.1883(1)
63	Neg	C48H71O21, 822+Glu		983.4456 (5.45E7)	821.3928(100: 1.83E6), 803.3832(35), 785.3726(1), 759.3929(2), 645.3619(5), 627.3516(2), 537.3564(1), 351.0555(12)
64	Pos	C32H47O5	17.75	511.3412 (1.49E6)	493.3298(35), 451.3196(95), 433.3091(40), 405.3142(100: 1.77E5), 387.3035(20), 361.2877(7), 189.1628(10)
65	Pos	C44H65O18		881.4150 (2.96E6)	705.3836(20), 529.3517(5), 511.3412(100: 1.38E6), 493.3305(1.5), 451.3205(2.5), 433.3096(1), 405.3153(2)

表1 LC-MS/MS測定により得られたカンゾウの成分情報(4)

No	極性	推定組成	保持時間	プリカーサ質量(強度)	プロダクト質量(相対強度)
66	Pos	C50H75O22, 703+2Glu		1027.4722 (4.20E6)	529.3522(30), 511.3413(100: 4.05E4)
	Neg	C50H73O22, 703+2Glu	17.98	1025.4562 (2.72E7)	1025(100: 4.00E6), 1007.4453(10), 921.4470(1), 891.4343(2), 861.3885(1), 703.3670(3), 643.3464(4), 625.3362(1), 581.3457(1), 497.1131(70), 479.1026(1), 453.1237(2), 435.1129(10), 407.1182(3), 339.0919(10), 321.0815(10)
67	Pos	C32H47O5	18.15	511.3388 (5.91E6)	493.3307(40), 451.3203(95), 433.3098(50), 405.3149(100: 8.53E5), 387.3044(20), 361.2887(6), 189.1631(8)
68	Pos	C44H65O18		881.4157 (3.41E7)	705.3839(15), 529.3516(7), 511.3412(100: 4.34E6), 493.3308(1), 451.3202(2.5), 433.3099(1), 405.3153(2)
	Neg	C44H63O18	18.35	879.3989 (1.53E8)	879(100: 1.27E6), 861.3888(4), 817.3986(3.5), 757.3776(3.5), 703.3674(3), 643.3463(2), 625.3359(1.5), 581.3464(1), 351.0555(30), 289.0553(2)
69	Pos	C15H13O4, 418-Glu	18.5	257.0812 (1.81E7)	242.0566(30), 239.0695(80), 229.0851(4), 211.0746(30), 163.0381(10), 147.0432(95), 137.0225(100: 1.14E6), 119.0484(6)
70	Pos	C21H21O6, GlyC+O		369.1333 (4.13E6)	351.1235(10), 341.1389(2), 313.0714(4), 285.0764(2), 205.0859(20), 193.0494(100: 1.07E6), 189.0909(20), 165.0544(90), 137.0594(20)
71	Pos	C42H61O17, 822+O-2H	18.85	837.3871 (6.90E6)	819.3788(1.5), 801.3687(1), 661.3579(4), 643.3476(20), 625.3371(40), 485.3260(100: 1.13E6), 467.3156(65), 449.3049(10)
72	Pos	C16H13O4, LicochalconB-H2O	18.92	269.0811 (4.92E6)	269(20), 254.0576(100: 4.58E5), 237.0547(50), 213.0910(45), 163.0387(4), 151.0386(3), 136.0151(6), 118.0410(7), 107.0489(8)
73	Pos	C50H79O21, 822+Glu+C2H4+2H	18.95	1015.5099 (2.95E6)	869.4515(90), 689.3886(20), 677.4251(10), 671.3782(30), 611.3570(80), 593.3476(5), 585.3512(15), 513.3570(5), 495.3462(15), 453.3359(100: 2.04E5), 435.3254(40), 423.3220(3), 407.3307(12), 395.2949(4), 389.3202(6)
74	Neg	C48H73O20, SS- I +2O-4H	18.97	969.4696 (1.98E6)	968(80), 951.4557(15), 907.4662(5), 835.4454(2), 805.3990(2), 647.3777(7), 497.1133(100: 3.89E5), 479.1025(2), 453.1237(2), 435.1130(12), 407.1181(3), 381.1024(1.5), 351.0554(2), 339.0919(15), 321.0815(15)
75	Neg	C48H69O22, 822+O-2H+Glu	19.01	997.4271 (1.21E6)	997(20), 979.4136(15), 953.4349(1.5), 935.4244(4), 891.4000(1), 863.4038(1.5), 833.3569(2), 675.3359(6), 497.1131(100: 3.35E5), 479.1027(2), 453.1234(2), 435.1129(8), 407.1180(4), 339.0919(12), 321.0815(12)
76	Pos	C50H77O22, 882+Glu-O	19.04	1029.4836 (1.38E7)	883.4302(100: 2.04E5), 865.4178(5), 707.3972(5), 689.3888(15), 671.3773(10), 611.3568(35), 495.3462(8), 453.3358(60), 435.3254(20)
77	Neg	C18H15O4, LicochalconB+O-2H	19.11	271.0965 (4.46E6)	271(95), 256.0730(70), 253.0860(70), 229.0861(30), 212.0834(10), 147.0448(100: 2.77E5), 135.0448(98), 123.0449(15), 109.0295(90)
73	Neg	C50H77O21, 822+Glu+C2H4+2H		1013.4937 (3.24E6)	1013(70), 995.4809(30), 951.4910(40), 909.4807(70), 867.4342(7), 823.4449(2), 805.4343(10), 781.4342(10), 763.4238(60), 745.4134(15), 687.3720(25), 669.3616(5), 645.3617(100: 6.25E5), 625.3727(1), 619.3624(3), 611.3574(1), 601.3721(15), 597.3772(12), 583.3616(5), 569.3463(8), 557.3459(2), 529.3516(5), 511.3411(5), 487.3410(15), 469.3305(30)
					835(50), 817.3619(10), 791.3826(2), 773.3723(5), 701.3528(1), 659.3411(14), 351.0555(100: 1.74E6), 333.0450(2), 289.0552(3)
74	Neg	C42H59O17, 822+O-2H	19.18	835.3725 (1.41E7)	835(50), 817.3619(10), 791.3826(2), 773.3723(5), 701.3528(1), 659.3411(14), 351.0555(100: 1.74E6), 333.0450(2), 289.0552(3)
76	Neg	C50H75O22, 882+Glu-O	19.28	1027.4715 (4.32E7)	No fragment
78	Pos	C48H71O20, SS- I +2O-8H	19.65	967.4499 (1.60E6)	949.4404(17), 821.3932(4), 803.3824(10), 645.3617(5), 469.3303(15), 451.3198(100: 3.34E5), 433.3093(4)
79	Pos	C44H67O18	19.84	883.4306(1.21E7)	689.3903(6), 671.3795(13), 653.3685(1), 629.3687(4), 611.3586(50), 593.3476(4), 585.3527(5), 529.3524(1), 513.3581(4), 495.3473(15), 471.3475(5), 453.3369(100: 1.44E6), 435.3265(40), 407.3315(10), 389.3210(6), 353.0722(4), 317.0512(4)
78	Neg	C48H69O20, SS- I +2O-8H	19.95	965.4352 (1.40E7)	965(100: 1.63E6), 947.4243(10), 921.4448(1.5), 903.4350(4), 831.4135(2), 801.3673(1.5), 643.3463(5), 497.1131(95), 479.1027(2), 453.1235(4), 435.1129(15), 407.1181(5), 381.1027(2), 339.0919(17), 321.0815(18)
80	Pos	C42H61O16	19.96	821.3930 (2.19E7)	803.3863(20), 645.3636(8), 469.3323(35), 451.3218(100: 2.31E6), 433.3112(2.5), 407.2957(1)
81	Pos	C42H63O17, 822+O	20.08	839.4055 (5.54E7)	821.3977(2), 803.3878(2), 663.3760(12), 645.3654(23), 627.3547(30), 487.3434(100: 9.93E6), 469.3330(90), 451.3224(15), 439.3223(2)
79	Neg	C44H65O18	20.11	881.4140 (2.76E7)	881(98), 863.4034(15), 820.4169(3), 819.4139(7), 747.3931(1), 705.3827(17), 687.3731(1), 645.3618(1), 487.3415(1), 351.0555(100: 2.72E6), 333.0450(2), 289.0554(2.5)
80	Neg	C42H59O16	20.21	819.3784 (8.50E7)	819(12), 801.3662(10), 775.3868(2), 757.3768(10), 643.3458(12), 625.3357(2), 351.0555(100: 3.43E6), 333.0449(2), 307.0659(1), 289.0554(6)
81	Neg	C42H61O17, 822+O	20.39	837.3889 (1.17E8)	837(50), 819.3776(15), 793.3984(2), 775.3879(6), 703.3675(1), 685.3571(1), 681.3568(15), 643.3466(5), 485.3257(2), 351.0555(100: 2.43E6), 333.0452(2), 289.0554(2.5)
82	Pos	C42H63O16	20.45	823.4110 (2.20E6)	647.3779(30), 471.3461(5), 453.3356(100: 1.20E6), 435.3251(2), 407.3304(2.5)
83	Pos	C44H65O18		881.4160 (5.41E6)	803.3859(3), 785.3756(4), 687.3745(10), 669.3645(60), 627.3530(10), 609.3434(90), 591.3321(3), 563.3379(6), 511.3424(100: 3.17E5), 493.3318(25), 469.3321(35), 451.3216(95), 433.3111(40), 405.3163(15), 393.2801(10), 387.3056(3), 353.0727(2)

表1 LC-MS/MS測定により得られたカンゾウの成分情報(5)

No	極性	推定組成	保持時間	プリカーサ質量(強度)	プロダクト質量(相対強度)
84	Pos	C48H73O20, SS- I +2O-6H		989.4681 (3.26E6)	951.4563(4), 933.4459(2), 823.4093(10), 689.3890(6), 647.3784(25), 495.3462(3), 471.3465(20), 453.3360(100: 4.63E5), 435.3257(2.5), 407.3310(3)
85	Pos	C21H21O5	20.46	353.1385 (1.12E6)	
86	Pos	C44H65O17, 822+C2H2O	20.52	865.4180 (7.37E6)	689.3889(15), 513.3568(4), 495.3462(100: 1.44E6), 477.3362(1), 435.3256(2), 417.3149(1)
87	Neg	C50H75O21, 822+Glu+C2H4	20.56	1011.4765 (1.85E7)	1011(60), 993.4659(15), 967.4863(1.5), 949.4757(5), 877.4549(1.5), 847.4088(2), 689.3881(5), 629.3668(1), 497.1132(100: 2.37E6), 479.1025(2), 453.1237(2.5), 435.1129(12), 407.1181(4), 381.1024(1), 339.0919(15), 321.0815(15)
88	Pos	C21H21O6, GlyC+O	20.62	369.1334 (4.29E6)	341.1390(1.5), 313.0714(100: 1.38E6), 301.0714(15), 169.0494(3)
89	Pos	C21H23O6, Glyasperin B	20.62	371.1489 (1.71E6)	
83	Neg	C44H63O18	20.7	879.3984 (1.13E7)	879(100), 861.3881(15), 835.4088(3), 817.3983(7), 745.3780(1), 703.3672(17), 685.3563(2), 351.0556(100: 2.00E6), 333.0450(2), 289.0553(2.5)
84	Neg	C48H71O20, SS- I +2O-6H		967.4505 (2.08E7)	967(90), 949.4398(15), 923.4614(1.5), 905.4500(5), 833.4288(2), 803.3821(1.5), 715.4028(1), 645.3618(8), 627.3516(2.5), 537.3563(1), 497.1131(100: 3.55E6), 479.1024(2), 453.1164(4), 435.1129(15), 407.1181(5), 381.1023(1), 339.0919(17), 321.0814(20)
86	Neg	C44H63O17, 822+C2H2O	20.79	863.4044 (1.94E7)	863(90), 845.3928(15), 819.4136(3), 801.4033(10), 729.3830(1), 687.3723(15), 669.3617(1), 351.0555(100: 1.59E6), 333.0450(2), 289.0554(4)
87	Pos	C42H63O16, Glycyrrhizin	20.96	823.4103 (6.03E7)	805.4017(1), 647.3802(10), 471.3478(13), 453.3373(100: 3.27E6), 435.3272(2), 407.3320(2.5), 389.3214(0.5)
	Neg	C42H61O16, Glycyrrhizin	21.14	821.3946 (2.54E8)	821(30), 803.3818(15), 777.4028(2), 759.3923(15), 687.3720(1), 645.3615(9), 627.3512(8), 537.3558(1.5), 469.3308(2), 351.0555(100: 1.58E7), 333.0451(2), 307.0659(1), 289.0553(7)
88	Pos		21.31	353.1886 (1.00E6)	338.1151(10), 297.0759(100: 6.78E5), 285.0758(15), 267.0652(30), 199.0750(5)
89	Pos	C42H65O15, 822- O+2H	22.22	809.4305 (5.20E6)	633.4008(25), 611.3587(15), 453.3375(20), 439.3580(100: 1.99E5)
90	Pos	C42H63O16		823.4096 (2.95E6)	647.3806(17), 609.3428(7), 471.3483(3), 453.3375(100: 6.01E5), 433.3115(4)
91	Pos	C30H45O3	22.25	453.3361 (1.24E6)	435.3251(100: 1.63E5), 407.3303(80), 389.3198(30), 266.2003(10), 235.1685(50), 217.1579(20), 189.1630(30), 175.1472(20)
92	Pos	C48H75O20, SS- I +2O-4H		971.4821 (2.37E6)	825.4248(100: 5.45E5), 807.4143(7), 789.4033(2), 649.3934(3), 631.3824(30), 619.4186(7), 613.3723(30), 567.3671(4), 455.3511(40), 437.3407(50), 409.3460(5), 397.3094(4), 353.0708(3), 317.0506(3)
89	Neg	C42H63O15, 822- O+2H	22.55	807.4162 (1.18E7)	807(40), 789.4034(15), 763.4246(3), 673.3934(1), 631.3829(13), 583.3627(1), 351.0556(100: 1.28E6), 333.0451(2), 289.0555(3)
90	Neg	C42H61O16		821.3939 (1.77E7)	821(20), 803.3826(10), 777.4035(3), 759.3928(7), 645.3620(10), 627.3518(5), 583.3621(2), 351.0555(100: 1.82E6), 333.0451(2), 289.0553(3)
93	Pos	C20H23O6, Licopyranocoumarin	22.57	359.1492 (1.64E6)	341.1398(2), 303.0869(100: 6.75E5), 249.1126(4), 221.1174(8)
94	Pos	C20H17O6	22.6	353.1024 (7.52E6)	335.0921(100: 1.47E6), 325.1077(15), 311.0555(20), 307.0971(45), 297.0399(10), 227.0703(25), 201.0909(10), 187.0752(7), 153.0179(70)
	Neg	C20H15O6	22.63	351.0863 (4.49E6)	336.0623(60), 333.0753(100: 1.81E5), 323.0911(30), 307.0963(30), 293.0807(10), 283.0964(10), 265.0859(15), 241.0860(5), 201.0187(7), 177.0190(7)
92	Neg	C48H73O20, SS- I +2O-4H		969.4686 (4.26E6)	969(50), 951.4548(20), 907.4648(5), 835.4446(1), 805.3973(2), 647.3771(5), 497.1129(100: 1.01E6), 479.1024(2), 453.1231(1), 435.1127(10), 407.1178(4), 339.0919(15), 321.0815(14)
93	Pos	C21H21O6, GlyC+O	22.64	369.1335 (2.60E7)	341.1393(15), 327.1236(20), 313.0717(100: 5.49E6), 299.1286(10), 285.0765(60), 191.1067(4), 149.0232(2)
	Neg	C21H19O6, GlyC+O	22.66	367.1175 (1.65E7)	367(30), 352.0936(10), 339.1221(3), 323.1273(4), 309.0391(100: 6.45E6), 297.0393(40), 284.0316(15), 203.0708(3), 148.0164(1)
94	Pos	C42H63O16	22.76	823.4086 (2.60E6)	805.3995(5), 787.3893(3), 769.3785(2), 647.3782(7), 629.3676(17), 611.3572(70), 565.3512(4), 471.3464(6), 453.3360(100: 6.47E5), 453.3254(40), 407.3309(7), 317.0506(4)
95	Pos	C48H77O19, SS- I +O-2H		957.5022 (9.26E6)	939.4964(2), 811.4497(100: 1.42E6), 793.4385(5), 775.4283(3), 757.4175(2), 635.4175(4), 617.4066(20), 599.3960(40), 581.3851(10), 441.3741(35), 423.3636(30), 405.3530(5), 335.0728(3), 317.0516(2)
96	Pos	C21H23O5, LicochalconeD	22.92	355.1542 (3.47E6)	313.1440(8), 299.0920(100: 2.08E6), 287.0919(6), 261.1123(2), 245.1173(2), 235.0964(1.5), 215.1066(1), 191.1065(10), 153.0544(6), 121.0282(3)
97	Neg	C50H75O21, 822+Glu+C2H4	22.92	1011.4764 (4.25E6)	1011(50), 993.4661(20), 967.4873(2), 949.4764(4), 905.4518(1), 877.4556(1.5), 847.4088(1.5), 689.3882(6), 497.1133(100: 9.80E5), 479.1026(2), 453.1237(2.5), 435.1130(10), 407.1181(3), 381.1026(1), 339.0920(13), 321.0815(12)
98	Neg	C21H21O5	22.96	353.1382 (1.73E6)	353(35), 338.1144(100: 5.74E5), 321.1119(70), 310.0833(5), 295.0600(12), 284.0679(15)

表1 LC-MS/MS測定により得られたカンゾウの成分情報(6)

No	極性	推定組成	保持時間	ブリカーサ質量(強度)	プロダクト質量(相対強度)
99	Pos	C21H25O5	23.05	357.1699 (3.48E6)	341.1381(1), 301.1065(100: 1.76E6), 289.1066(10), 247.1322(3), 235.1322(30), 221.1165(50), 179.0695(2), 153.0538(1.5), 123.0434(3.5)
100	Pos	C42H63O16		823.4088 (9.25E6)	805.3996(2), 787.3889(3), 769.3789(1), 647.3782(2), 629.3674(20), 611.3569(70), 565.3513(10), 453.3358(100: 1.92E6), 435.3253(40), 407.3305(10), 395.2942(7), 353.0715(3), 317.0503(5)
101	Neg	C21H23O5, GlyC+4H	23.08	355.1538 (2.40E6)	337.1430(10), 323.1275(100: 7.13E5), 286.0835(10), 279.1380(10), 254.0575(15), 245.1174(15), 233.1174(20), 219.1019(15), 207.1020(18), 147.0450(2)
95	Neg	C48H75O19, SS- I +O-2H		955.4900 (1.56E7)	955(40), 937.4762(20), 893.4868(5), 821.4662(1), 791.4188(1), 633.3984(7), 497.1132(100: 4.09E5), 479.1027(2), 453.1237(1), 435.1130(8), 407.1181(3), 381.1023(1), 339.0919(15), 321.0814(15)
100	Neg	C42H61O16	23.2	821.3965 (5.15E6)	821(13), 803.3825(15), 777.4037(3), 759.3931(8), 687.3727(1), 645.3619(20), 627.3517(3), 469.3303(2), 351.0555(100: 2.88E5), 333.0450(3), 289.0554(3)
102	Pos	C20H19O6, GlycyrdioneA+O-2H	23.34	355.1178 (3.68E6)	337.1062(1), 299.0542(100: 1.91E6), 287.0541(40)
	Neg	C20H17O6, GlycyrdioneA+O-2H	23.26	353.1017 (3.54E6)	353(70), 300.0365(10), 310.0470(10), 298.0468(100: 3.81E5), 284.0315(70)
103	Pos	C42H65O16	23.4	825.4241 (1.23E7)	807.4178(2), 789.4071(2), 771.3969(1.5), 631.3854(15), 613.3751(60), 567.3690(10), 455.3531(70), 437.3426(100: 1.19E6), 409.3477(20), 397.3113(10), 365.1972(2), 353.0728(5), 335.0621(3), 317.0515(8)
104	Neg	C42H61O16	23.43	821.3933 (1.77E7)	821(90), 803.3823(15), 777.4029(2), 759.3925(6), 687.3722(1), 645.3616(12), 627.3511(1.5)< 469.3304(1), 351.0555(100: 2.08E6), 333.0450(2), 289.0553(2.5)
105	Pos	C21H21O5, Glycycomarin (GlyC)	23.69	353.1387 (2.08E6)	335.0921(100: 1.47E6), 325.1077(10), 311.0555(20), 307.0971(45), 297.0399(10), 227.0703(25), 201.0909(10), 187.0752(7), 153.0179(70)
103	Neg	C42H63O16	23.81	823.4096 (2.11E7)	823(30), 805.3981(10), 779.4191(3), 761.4086(5), 689.3875(1), 647.3776(13), 629.3673(1), 471.3464(1), 351.0555(100: 1.30E6), 333.0451(2), 289.0554(3)
104	Pos	C20H19O5, GlycyrdioneA-2H	23.91	339.1231 (3.21E6)	311.1273(100: 1.40E6), 284.0674(30), 189.0903(20)
105	Pos	C30H45O2		437.3410 (1.70E6)	419.3308(20), 331.2791(20), 367.23318(15), 339.2318(20), 313.2162(50), 285.1847(100: 1.00E5), 269.2262(30), 255.2105(60), 215.1790(20), 201.1632(25), 189.1633(30), 163.1476(35)
106	Neg	C20H19O5, GlycyrdioneA	23.93	339.1226 (2.65E6)	324.0988(100: 1.81E6), 309.1119(7), 281.0444(5), 269.0444(7)
107	Pos	C20H19O6, GlycyrdioneA+O-2H	23.97	355.1179 (2.23E6)	337.1079(35), 327.1235(20), 313.0715(5), 299.0557(100: 9.20E5), 287.0555(10), 229.0861(20), 201.0910(5), 189.0909(30), 179.0338(15), 151.0387(15)
108	Neg	C48H73O19, SS- I +O-4H	23.97	953.4708 (2.14E6)	953(40), 935.4600(15), 909.4802(1), 891.4704(4), 819.4493(1), 789.4029(2), 631.3823(5), 613.3722(1), 497.1129(100: 4.80E5), 479.1023(2), 453.1235(2), 435.1128(12), 407.1180(5), 381.1024(2), 339.0919(15), 321.0814(18)
109	Pos	C21H23O5, Licochalcon D	24.1	355.1542 (1.89E6)	337.1080(3), 327.1237(2), 299.0922(100: 1.51E6), 287.0557(5), 233.1175(8), 221.1174(17), 189.0909(3), 177.0545(2), 147.0438(1.5), 123.0439(2)
110	Neg	C42H61O15	24.26	805.3987 (1.49E7)	805(40), 787.3878(15), 761.4091(3), 743.3984(7), 629.3672(10), 611.3564(2), 567.3663(0.5), 521.3618(0.7), 453.3359(0.8), 351.0556(100: 2.06E6), 333.0450(2), 289.0553(3), 261.0606(1)
111	Pos	C21H23O4, LicochalconA	24.29	339.1594 (8.93E5)	
112	Pos	C20H21O5, GlycyrdioneA	24.3	341.1387 (1.66E6)	298.1523(10), 285.0761(100: 8.27E5), 267.0654(50), 249.0548(4), 221.0598(5), 215.1066(6), 179.0337(55), 153.0179(10)
113	Pos	C20H19O6, GlycyrdioneA+O-2H		355.1178 (3.07E6)	299.0555(85), 287.0554(100: 6.25E5)
	Neg	C20H17O6, GlycyrdioneA+O-2H	24.34	353.1020 (2.33E6)	353(40), 325.1065(6), 310.0468(12), 297.0392(100: 8.82E5), 284.0315(6), 240.0418(2), 151.0035(2)
114	Pos	C22H23O6, Glycoricone	24.42	383.1490 (3.73E6)	327.0858(100: 3.03E6)
	Neg	C22H21O6, Glycoricone	24.42	381.1330 (1.48E6)	381(60), 366.1093(60), 351.0859(100: 4.48E5), 323.0547(95), 311.0549(20), 297.0393(10)
115	Neg	C48H75O18, SS- I -2H	24.46	939.4940 (4.01E6)	939(50), 921.4814(15), 895.5023(2), 877.4915(5), 805.4711(1), 775.4249(2), 617.4036(5), 497.1132(100: 3.15E5), 479.1029(2), 453.1235(3), 435.1129(13), 407.1181(5), 381.1025(1), 339.0919(17), 321.0815(17)
116	Pos	C21H19O6, GlyC+O-2H	24.62	367.1177 (6.26E6)	352.0948(5), 339.1232(25), 311.0555(100: 2.19E6), 283.0605(15), 267.0655(2)
117	Neg	C42H63O15	24.75	807.4164 (1.03E7)	808.4172(7), 789.4034(13), 763.4241(2), 745.4138(6), 631.3829(10), 613.3723(3), 523.3772(1), 455.3520(0.5), 351.0555(100: 1.31E6), 333.0450(2), 289.0554(3), 261.0606(1)
118	Pos	C36H55O10, 471+GluUA	24.87	647.3772 (1.11E6)	471.3471(2), 453.3369(100: 1.37E6)
	Neg	C36H53O10, 471+GluUA	25.07	645.3631 (1.39E6)	645(20), 627.3494(60), 583.3600(25), 569.3446(80), 565.3499(20), 541.3501(15), 523.3397(40), 511.3398(3), 497.3245(5), 469.3297(100: 1.70E5), 425.3405(2)

表1 LC-MS/MS測定により得られたカンゾウの成分情報(7)

No	極性	推定組成	保持時間	プリカーサ質量(強度)	プロダクト質量(相対強度)
119	Neg	C42H61O15		805.4004 (1.52E6)	787.3877(12), 761.4086(3), 629.3671(10), 351.0555(100: 2.25E5), 333.0449(2), 289.0554(3)
120	Neg	C21H19O5, Glycycomarin	25.16	351.1227 (9.03E5)	336.0986(100: 3.45E5), 308.1040(40), 291.0287(20), 281.0444(40), 216.0420(4)
121	Pos	C21H19O5, Glycycomarin-2H	25.17	351.1230 (3.17E6)	295.0605(100: 1.06E6), 265.0497(30)
122	Pos	C28H35O6, 409+CH2O+4H	25.85	443.2424 (9.42E5)	425.2332(100: 7.55E5), 369.1704(1.5)
	Neg	C28H33O6, 409+CH2O+4H	25.85	441.2272 (7.65E5)	409.2000(100: 2.45E5), 353.1377(20), 309.1483(5), 233.1174(18), 221.1174(30), 195.1020(15)
123	Neg	C42H61O16		821.3951 (2.62E5)	803.3806(10), 759.3926(7), 715.3672(7), 645.3618(17), 351.0555(100: 2.17E4)
124	Neg	C44H65O16, Glycyrrhizin+C2H4		849.4258 (4.74E5)	849(40), 831.4141(15), 787.4232(7), 673.3934(10), 351.0555(100: 4.92E4)
125	Pos	C22H23O6, Glycoricone	26.74	383.1491 (3.90E6)	341.1388(7), 327.0866(20), 299.0917(100: 8.01E5)
	Neg	C22H21O6, Glycoricone	26.76	381.1333 (1.71E6)	381(20), 366.1091(100: 6.56E5), 351.0859(80), 323.0547(4), 297.0392(7)
126	Pos	C25H29O6, GlyinflamineA+O	28.54	425.1956 (6.68E5)	369.1342(100: 3.22E5), 357.1342(10), 313.0714(15), 221.1171(5), 191.1066(13)
127	Pos	C28H33O5, GlyinflamineA+CH2+2H	28.6	425.2321 (6.60E6)	369.1703(100: 2.48E6), 357.1705(4), 313.0712(5), 221.1172(30), 191.1065(17)
126	Neg	C25H27O6, GlyinflamineA+O	28.57	423.1804 (2.80E5)	391.1896(20), 233.0810(100: 5.57E4), 229.0862(60), 193.0865(25)
127	Neg	C28H31O5, GlyinflamineA+CH2+2H	28.64	423.2168 (3.48E6)	391.1896(100: 7.09E5), 347.2000(25), 322.1196(17), 278.1301(10), 245.1174(15), 233.1174(15), 215.1070(20), 207.1020(15), 193.0865(7), 177.0917(10)
128	Pos	C22H23O5, Glycycomarin+CH2	28.8	367.1543 (2.01E6)	353.1389(80), 335.1283(20), 323.0919(20), 309.0762(100: 3.15E5), 297.0762(50), 257.1174(7), 233.1173(5), 189.0544(6), 177.0544(13), 165.0543(60), 147.0437(15)
129	Neg	C22H23O5, Glycoricone+O-2H	28.82	367.1540 (1.62E6)	352.1299(80), 337.1065(100: 2.04E5), 309.0754(60), 297.0756(20), 284.0679(4)
130	Pos	C25H29O5, Glyinflamin A	28.96	409.2008 (1.09E5)	
131	Neg	C50H77O20, SS- I +2CO	29.04	997.5028 (9.27E5)	997(100: 1.42E5), 979.4858(10), 675.4086(3), 497.1131(50), 435.1128(5), 339.0919(12), 321.0814(12), 299.1095(2)
132	Neg	C25H25O5, PrenyllicoflavoneA	31.39	405.1695 (3.22E5)	382.1039 (70), 361.1065(5), 350.1140(90), 307.0599(100: 9.36E4), 295.0600(35), 269.0807(3), 243.1381(6)
	Pos	C25H27O5, PrenyllicoflavoneA	31.4	407.1852 (4.32E5)	351.1234 (100: 5.44E5), 295.0603)

表2 LC-MS/MS測定により得られたニンジンの成分情報(1)

極性	推定組成	保持時間	プリカーサー質量(強度)	プロダクトイオン質量(相対強度)
Neg	C48H81O19, Ginsenoside M6a	11.83	961.5375 (1.12E5)	799.4843(90, -Glc), 637.4318(100: 1.03E4, -2Glc), 475.3789(55, -3Glc)
Pos	C48H82O19 + Na	11.83	985.5285	
Neg	C47H79O18	12.14	931.5274 (8.92E4)	799.4841(45, -Ara), 769.4731(20), 637.4312(100: 1.92E4, -Ara & Glc), 619.4207(15), 475.3787(30)
Neg	C42H71O14, Ginsenoside Rg1 (標準品と一致)	12.82	799.4855 (2.55E5)	637.4318(100: 5.02E4), 619.4214(5), 475.3788(25)
	C44H75O16(酢酸付加)		859.5068 (4.29E5)	799.4844(100: 2.42E5), 637.4317(15)
	C48H81O18, Ginsenoside Re		945.5433 (2.88E5)	799.4840(30), 783.4888(100: 3.80E4), 765.4783(25), 637.4313(95), 619.4208(35), 475.3787(50)
			1005.5647 (1.14E5)	
Pos	C48H83O18, Ginsenoside Re	12.93	947.5525	
	C30H47O		423.3621 (1.50E5)	
	C30H49O2		441.3725 (1.39E5)	
			621.4345 (5.46E4)	
			1601.9727 (3.95E4)	
Neg	C42H71O14	17.1	799.4836 (3.35E5)	637.4302(85, -Glc), 475.3781 (100: 1.55E4, -2Glc)
Pos		17.2	423.362	
			441.3725	
	C42H71O13		783.4855	
			1601.9718	
Neg	C41H69O13	17.75	769.4732 (1.57E5)	637.4310(100: 2.35E4, -Ara), 475.3786(80, -Ara & Glc)
	C41H70O16N		832.4684 (4.76E4)	
	C58H97O26		1209.6256 (4.78E4)	1077.5837(100: 1.19E4, -Xly), 945.5402(15, -2Xly), 783.4911(10)
Pos		17.85	423.3619	
			753.4751 (2.47E4)	
			1211.6313 (3.20E4)	
Neg	C54H91O23, Ginsenoside Rb1 (標準品と一致)	18.05	553.2938 (2価-, 1.30E5)	945.5417(100: 3.37E4), 783.4888(55), 765.4783(10)
	[N-H]-		1107.5953 (5.20E5)	
Pos		18.13	1109.6018 (1.32E5)	
Neg		18.54	604.3092 (4.47E4)	
	C53H89O22, Ginsenoside Rc		1077.5842 (1.85E5)	945.5405(100: 2.32E3), 783.4882(70)
	C58H97O26		1209.6264 8.28E4)	1077.5840(100: 3.68E4), 945.5414(20), 915.5319(10), 783.4884(7)
	C38H65O11		697.4528	637.4312(100: 4.04E4), 475.3786(10)

表2 LC-MS/MS測定により得られたニンジンの成分情報(2)

極性	推定組成	保持時間	プリカーサー質量(強度)	プロダクトイオン質量(相対強度)
Pos		18.7	1079.5920 (7.05E4)	
			1228.6580 (5.34E4)	
Neg	C48H75O19, Ginsenoside Ro	19.24	955.4907 (8.26E5)	793.4360(100: 2.77E4), 613.3734(12), 523.3782(15)
	[3M-2H] ²⁻		1433.7405 (2価-, 1.94E5)	1911.9877(40), 1434.7413(45), 955.4890(100: 1.05E5), 739.4359(13)
Pos		19.27	1079.5916	
			1096.6178	
Pos		19.48	439.3567 (7.15E4)	
			974.5259 (1.76E5)	
			1453.2664 (2.77E4)	
			1931.0004 (3.06E4)	
Neg	C48H81O18, Ginsenoside Rd	20.5	945.5418 (1.78E5)	783.4884(100: 2.09E4, -Glc), 621.4359(30, -2Glu), 459.3832(10, -3Glc)
			1008.5371 (4.82E4)	
Pos	C42H71O12	20.62	767.4918 (5.34E4)	
	C48H83O18, Ginsenoside Rd		947.5539 (1.28E4)	
			964.5805(4.83E4)	
Neg	C42H65O14	26.12	793.4373 (2.22E5)	613.3732(100: 1.07E4), 569.3829(35), 523.3781(60), 455.3519(20)
Pos	C42H70O14N (NH4付加)	26.31	812.4786 (4.95E4)	
Neg	C72H71O13, Ginsenoside Rg2	26.61	783.4888 (1.30E5)	
	C72H71O13, Ginsenoside Rg2	26.95	783.4894 (1.30E5)	621.4358 (100: 1.33E4), 459.3835(40)

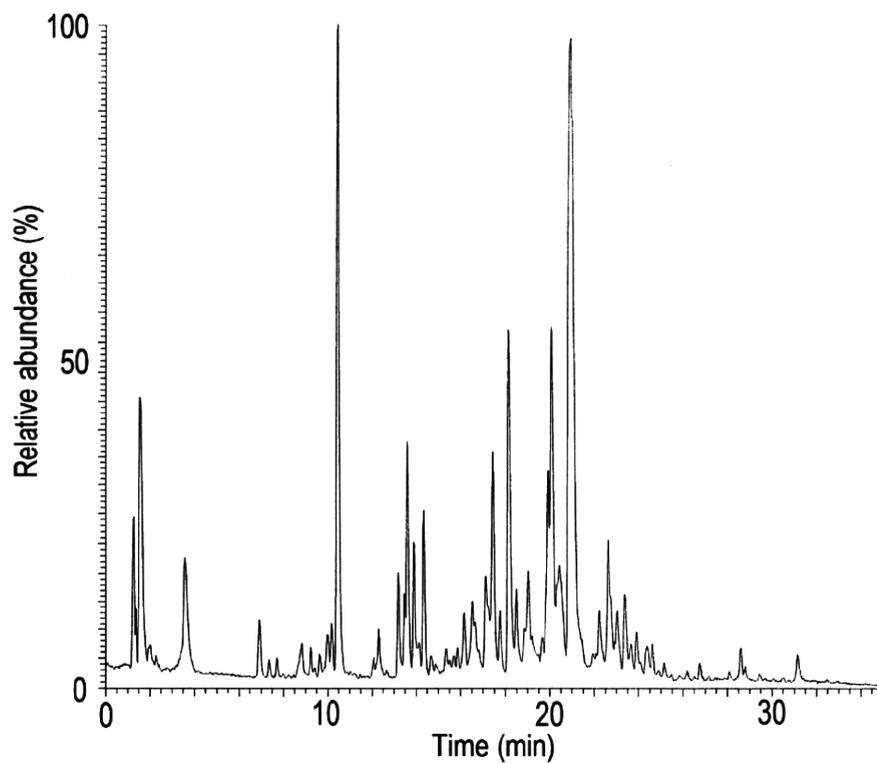


図 1 ポジティブイオン化モードにおける全イオンクロマトグラム(TIC)

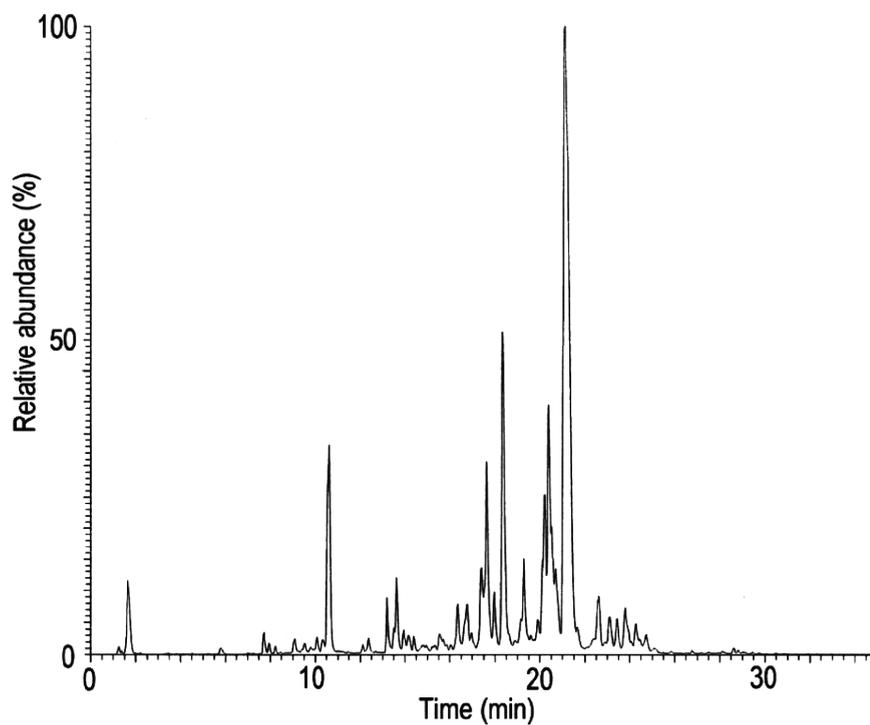


図 2 ネガティブイオン化モードにおける全イオンクロマトグラム(TIC)

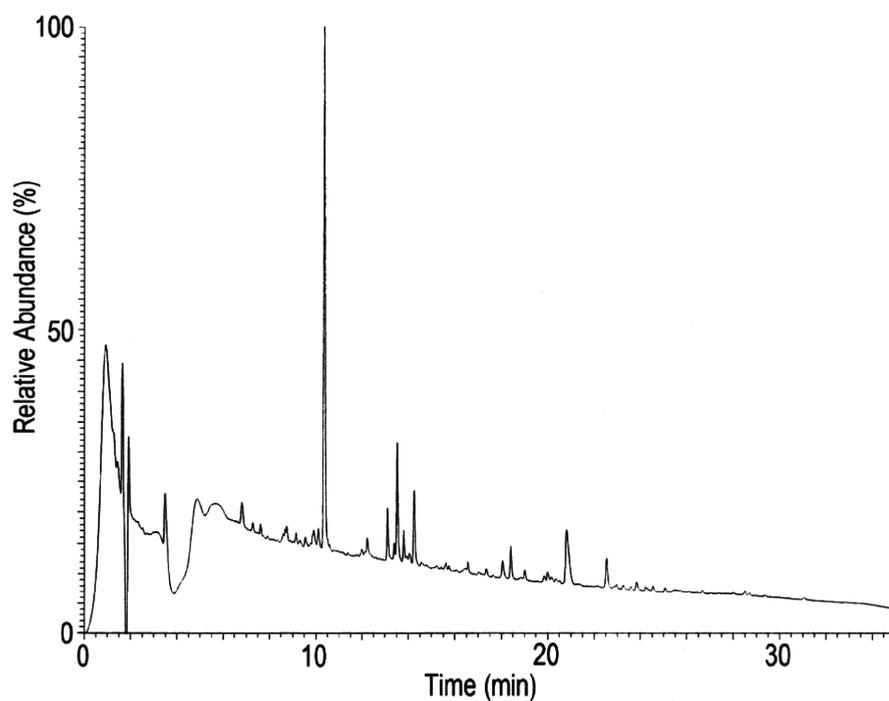


図 3 PDA による全波長クロマトグラム

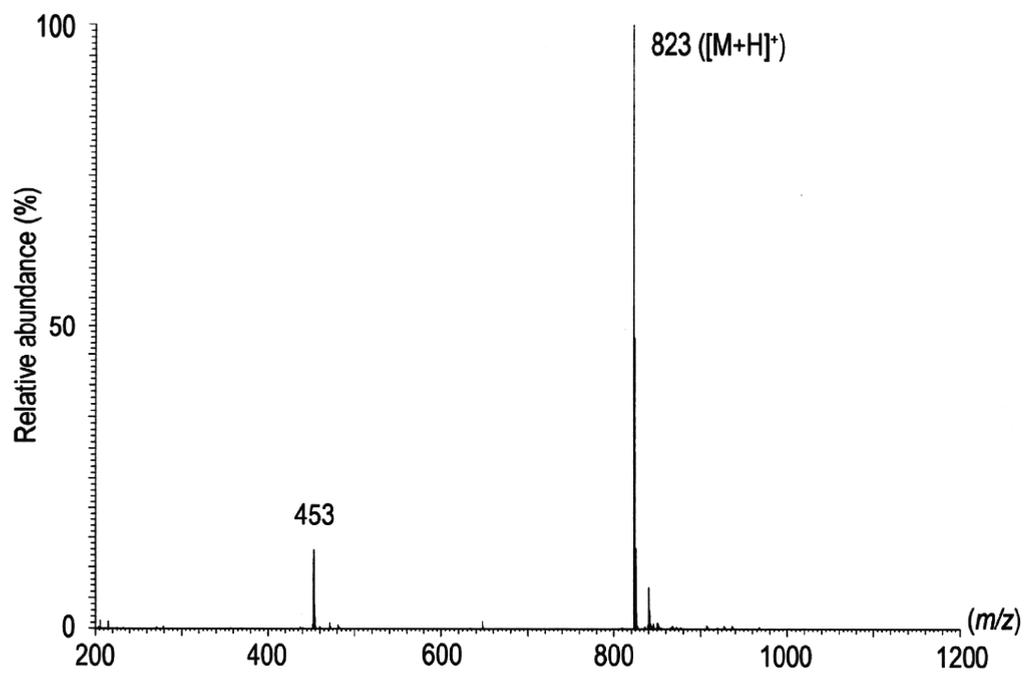


図 4 グリチルリチン (Rt 20.1 min) の MS (pos.)

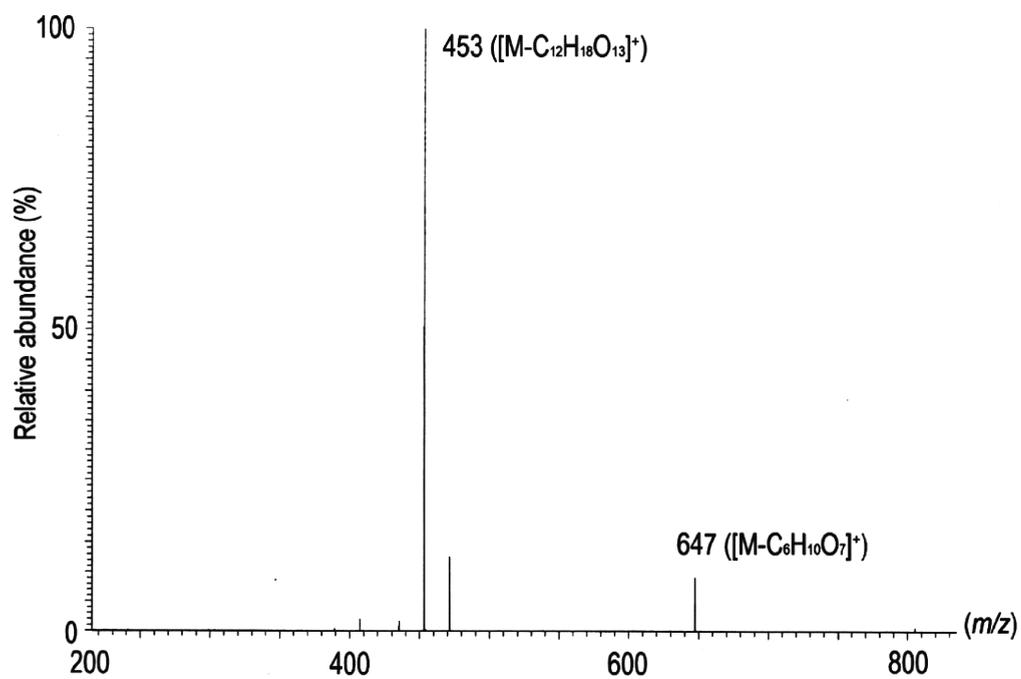


図 5 グリチルリチン (Rt 20.1 min) の MS/MS (pos., precursor m/z 823)

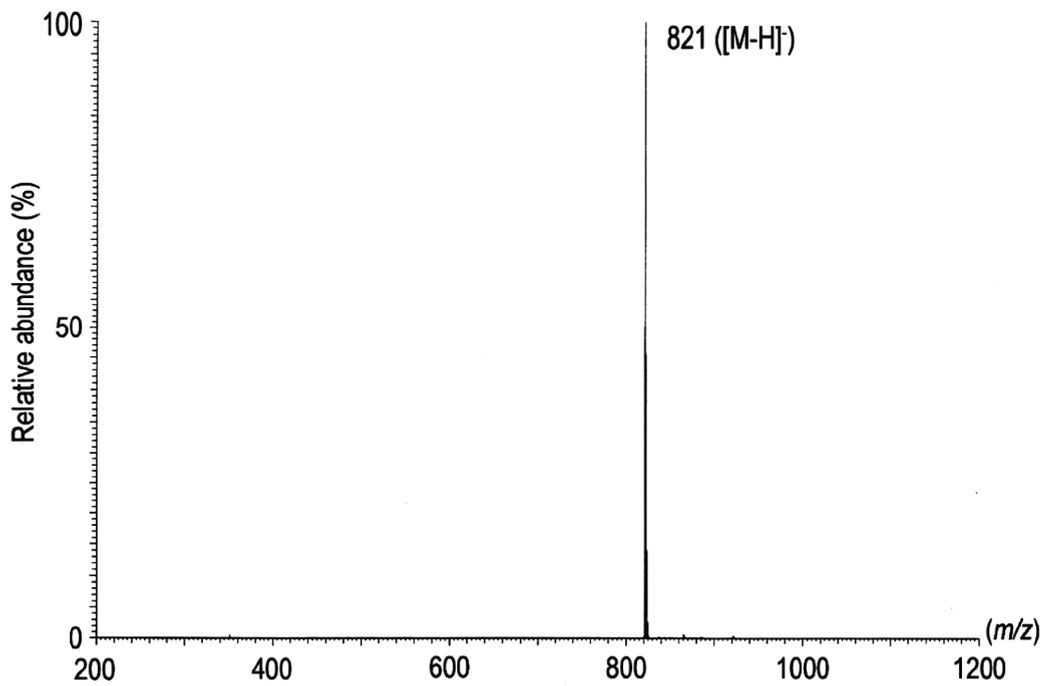


図 6 グリチルリチン (Rt 20.1 min) の MS (neg.)

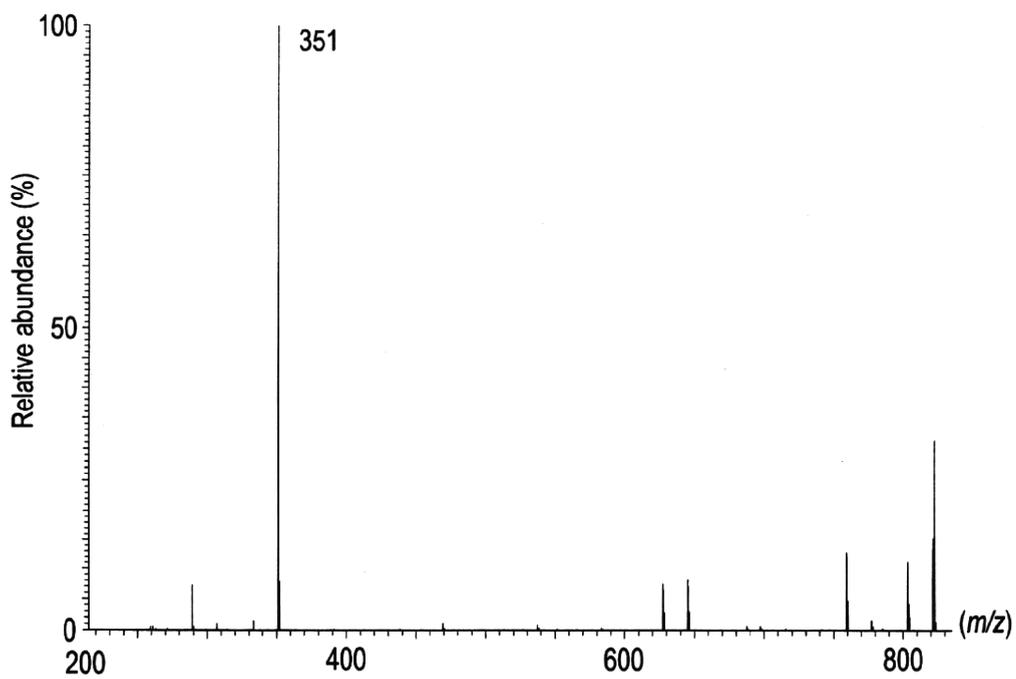


図 7 グリチルリチン (Rt 20.1 min) の MS/MS (neg., precursor m/z 821)

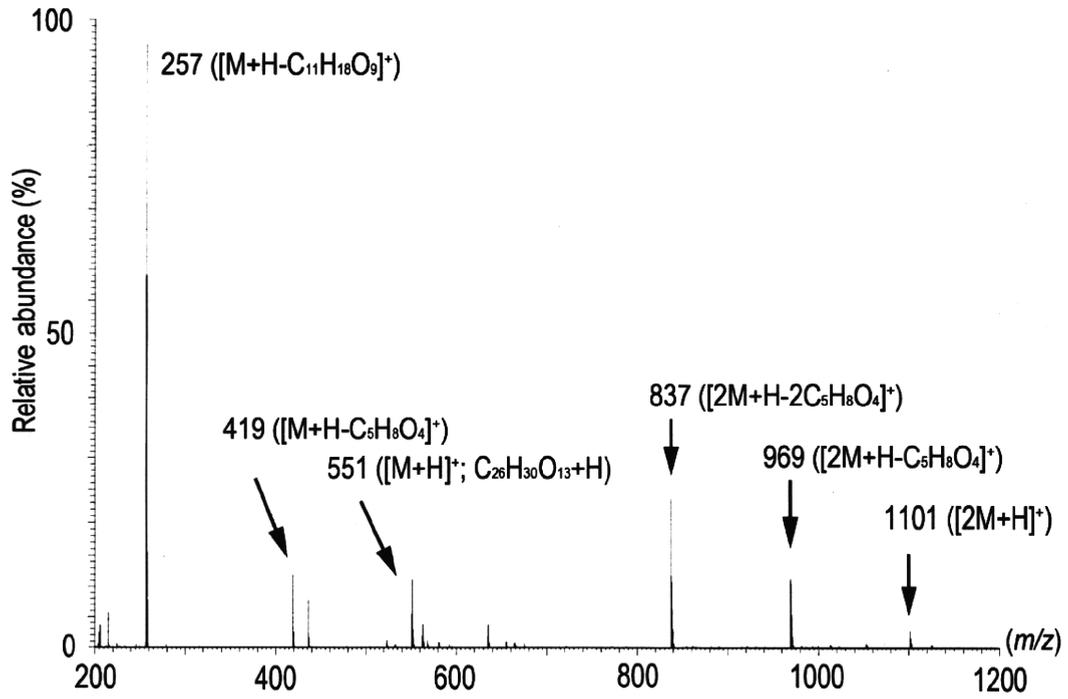


図 8 フラボノイド成分 (Rt 10.5 min) の MS (pos.)

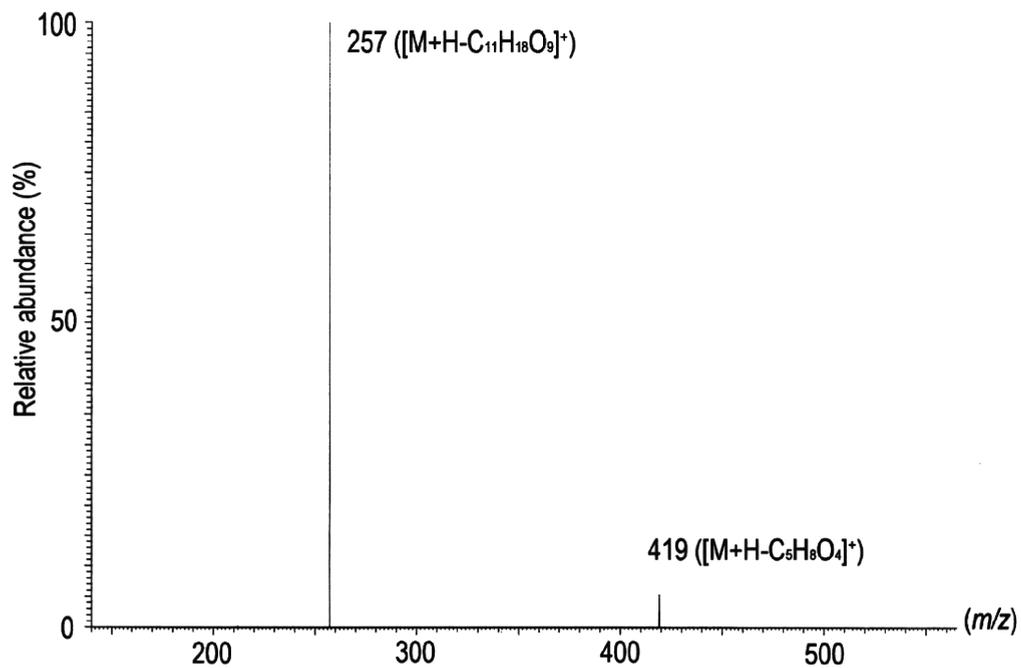


図 9 フラボノイド成分 (Rt 10.5 min) の MS/MS (pos., precursor m/z 551)

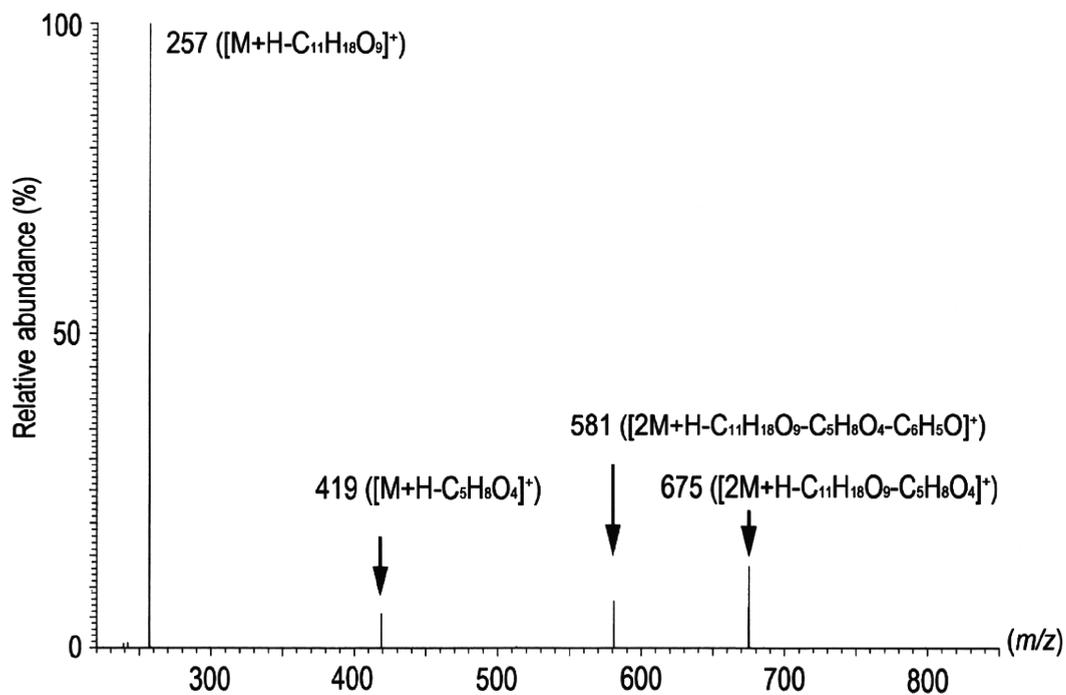


図 10 フラボノイド成分 (Rt 10.5 min) の MS/MS (pos., precursor m/z 837)

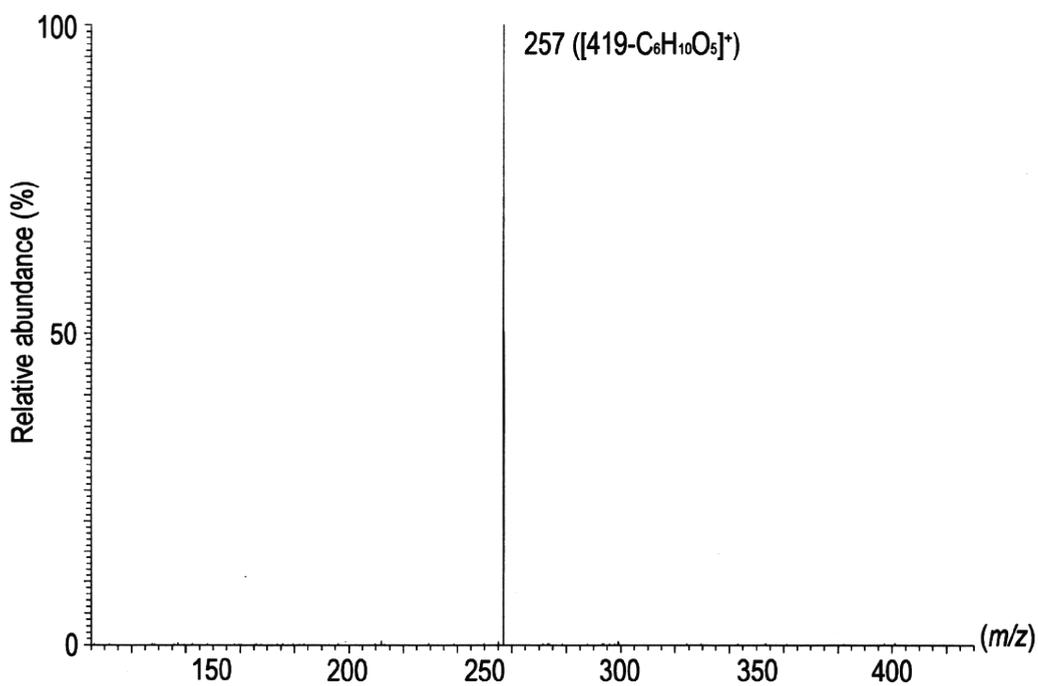


図 11 フラボノイド成分 (Rt 10.5 min) の MS/MS (pos., precursor m/z 419)

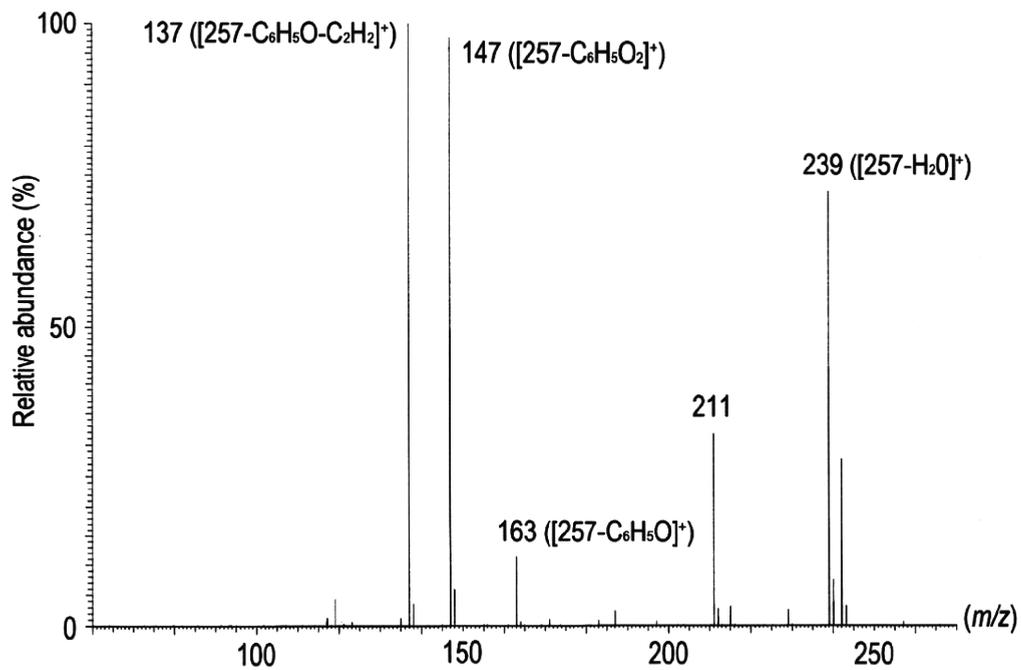


図 12 フラボノイド成分 (Rt 10.5 min) の MS/MS (pos., precursor m/z 257)

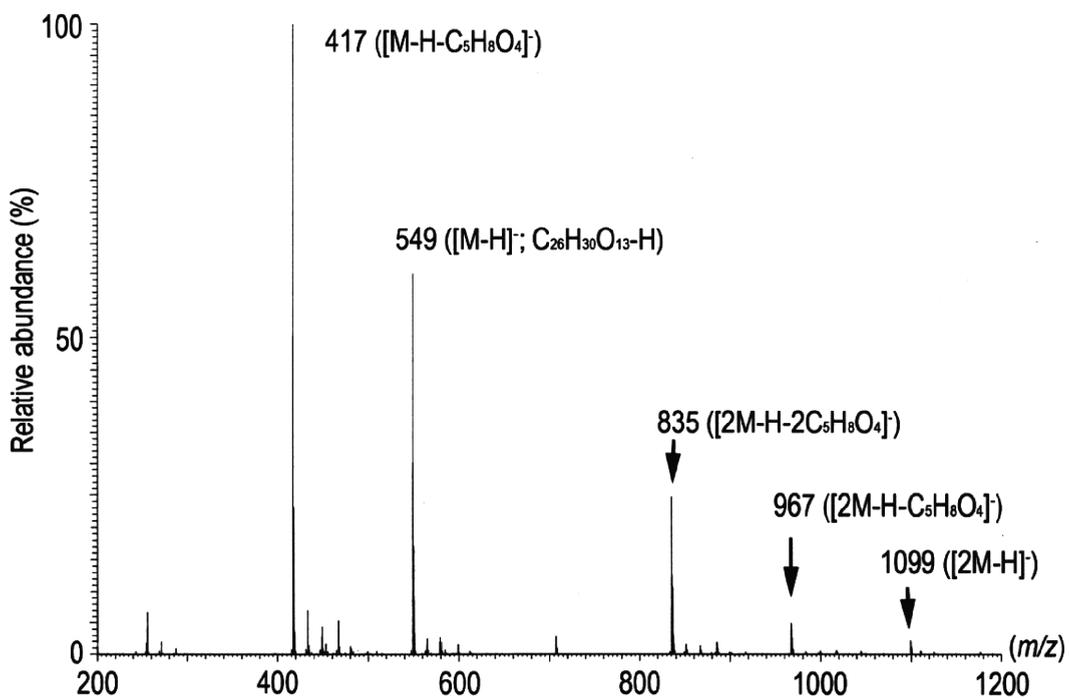


図 13 フラボノイド成分 (Rt 10.5 min) の MS (neg.)

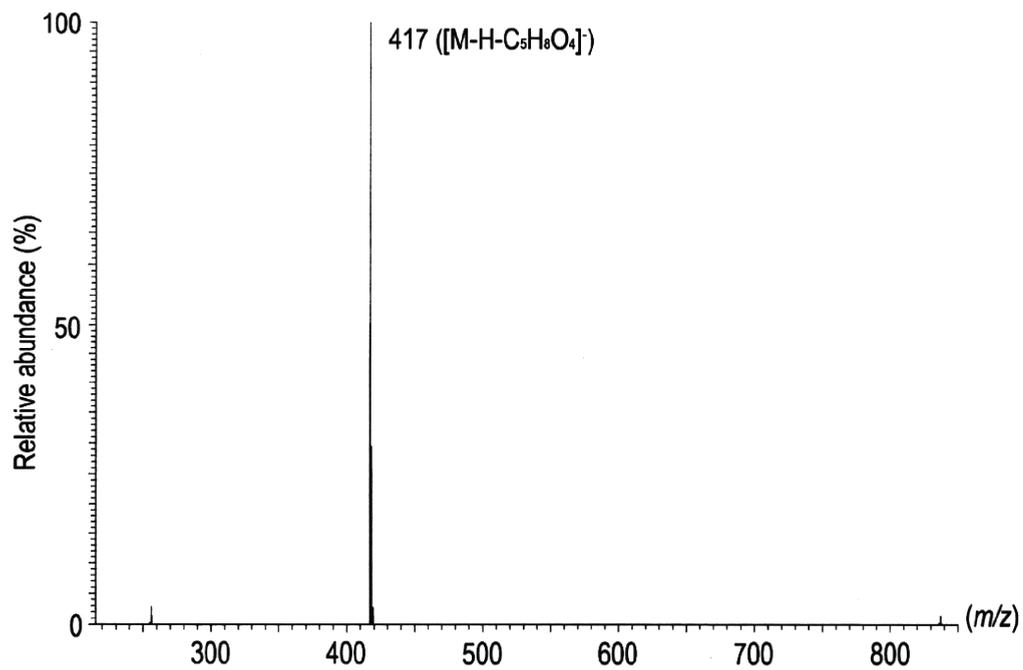


図 14 フラボノイド成分 (Rt 10.5 min) の MS/MS (neg., precursor m/z 835)

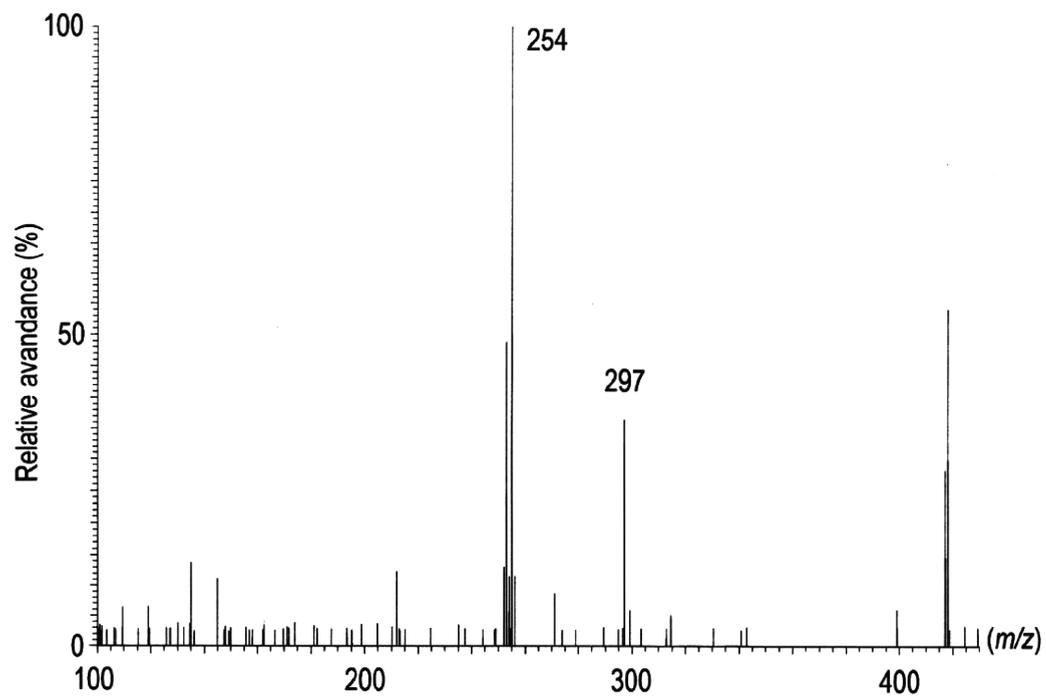


図 15 フラボノイド成分 (Rt 10.5 min) の MS/MS (neg., precursor m/z 549)

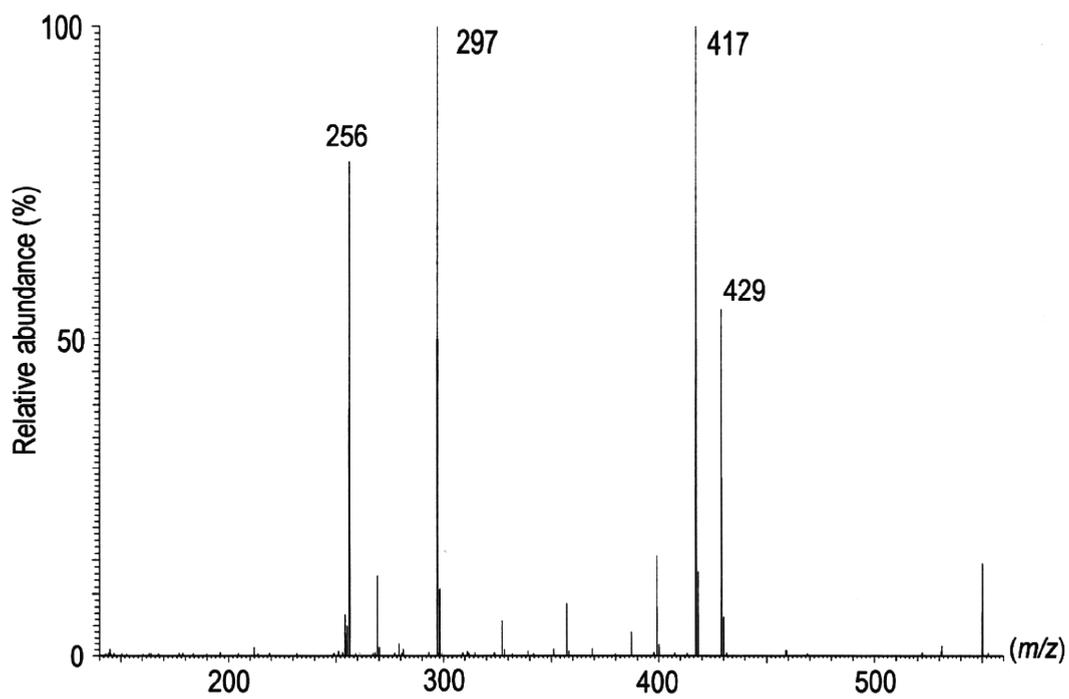


図 16 フラボノイド成分(Rt 10.5 min)の MS/MS (neg., precursor m/z 417)