

表1 キキョウのマススペクトルデータ(4)

8.89	205.0977 (5.31E6)	C11H13O2N2	188.0702(6.87E6; 100, C11H10O2N), 163.0177(3,)				
9.1	367.1503 (3.03E6)	C17H23O7N2	349.1393(4.32E5; 100, C17H21O6N2), 331.1287(20, C17H19O5N2), 271.1072(5, C15H15O3N2), 229.0966(15, C13H13O2N2)				
9.2	266.1140 (3.37E6)	C12H16O4N3	248.1025(2.95E6; 100, C12H14O3N3), 236.1025(25, C11H14O3N3),				
9.43	382.1498 (1.64E6)	C18H24O8N	364.1391(3.35E5; 100, C18H22O7N), 354.1548(10, C17H24O7N), 346.1285(12, C18H20O6N), 336.1441(7, C17H22O6N), 318.1333(3, C17H20O5N), 198.0756(5, C9H12O4N), 186.0757(50, C8H12O4N), 168.0652(15, C8H10O3N), 158.0809(15, C7H12O3N)				
10.48	382.1499 (5.68E6)	C18H24O8N	364.1390(9.35E5; 100, C18H22O7N), 354.1547(25, C17H24O7N), 346.1284(5, C18H20O6N), 336.1441(3, C17H22O6N), 318.1333(2, C17H20O5N), 258.0967(5, C11H16O6N), 198.0755(8, C9H12O4N), 186.0756(40, C8H12O4N), 168.0652(10, C8H10O3N), 158.0807(15, C7H12O3N)				
10.52	355.1028 (2.36E6)	C16H19O9	339.0394				
10.64	217.0976 (2.50E6)	C12H13O2N2	188.0701(3, C11H10O2N), 173.1068(15, C11H13N2), 171.0912(25, C11H11N2), 144.0804(1.43E6; 100, C10H10N)				
10.74	303.1344 (1.19E6)	C16H19O4N2	285.1232(1.06E6; 100, C16H17O3N2)				
11.09	303.1344 (8.56E5)	C16H19O4N2	285.1230(1.09E6; 100, C16H17O3N2), 195.0911(2, C13H11N2), 179.0697(2, C10H11O3)				
11.72	347.1241 (2.17E6)	C17H19O6N2	329.1130(6.45E5; 100, C17H17O5N2), 311.1024(90, C17H15O4N2), 293.0917(20, C17H13O3N2)				

表1 キキョウのマスペクトルデータ(5)

11.86	347.1241 (1.82E6)	C17H19O6N2	329.1132(4.67E5; 100, C17H17O5N2), 311.1025(50, C17H15O4N2), 293.0918(5, C17H13O3N2)				
12.58	310.1291 (2.10E7)	C15H20O6N	292.1176(2.76E5; 100, C15H18O5N), 282.1332(60, C14H20O5N), 264.1226(30, C14H18O4N), 221.0803(50, C12H13O4), 179.0697(20, C10H11O3), 114.0546(10, C5H8O2N)				
12.91	310.1293 (2.70E7)	C15H20O6N	292.1177(6.14E4; 100, C15H18O5N), 282.1332(60, C14H20O5N), 264.1227(30, C14H18O4N), 221.0803(50, C12H13O4), 177.0542(15, C10H9O3)				
				15.6	485.2237 (4.35E5)	C20H37O13 ([M+AcO]-)	425.2032(1.92E5; 100, C18H33O11 ([M-H]-)
				16.39	455.2128 (5.45E5)	C19H35O12 ([M+AcO]-)	395.1926(4.01E5; 100, C17H31O10 ([M-H]-)
18.69	1417.6470 (2.59E6)	C64H105O34 ([M+H]+)	1285.6067(60, C59H97O30: -Pen), 1123.5522(40, C53H87O25: 1285-Hex), 961.5001(30, C47H77O20: 1123-Hex), 845.4539(35, C42H69O17), 829.4584(70, C42H69O16: 961-Pen), 683.4007(3.08E3; 100, C36H59O12), 667.4055(75, C36H59O11: 829-Hex), 653.3885(40, C35H57O11), 521.3475(60, C30H49O7), 503.3369(65, C30H47O6), 485.3260(80, C30H45O5), 455.3155(70, C29H43O4)	18.74	737.3230 (2-, 1.55E6)	1475.6538 C66H107O36 ([M+AcO]-)	1005.4918(40, C48H77O22), 987.4813(3, C41H79O26), 707.3140(2-, 1.54E6; 100, C64H102O34: (M-2H]2-)), 409.1355(15, C16H25O12)
	1007.5045 (2.99E6)	C48H79O22	845.4525(40, C42H69O17: -Hex), 683.4007(2.80E5; 100, C36H59O12), 521.3469(60, C30H49O7), 503.3369(50, C30H47O6), 485.3258(55, C30H45O5), 455.3154(30, C29H43O4)				
18.93	1549.6890 (1.93E6)	C69H113O38	1417.6481(1.10E4; 100, C64H105O34: -Pen), 以下18.69分のm/z 1417と共通	18.99	773.3345 (2-, 3.77E6)	1547.6763 C69H111O38	1005.4916(1.74E6; 100, C48H77O22), 987.4816(15, C41H79O26), 728.3190(2-, 20,), 541.1779(20, C21H33O16), 469.1566(15, C18H29O14), 409.1353(5, C16H25O12)

表1 キキョウのマススペクトルデータ(6)

	1139.5468 (1.87E6)	C53H87O26	1007.5057(20, C48H79O22: -Pen), 977.4948(25, C47H77O21), 845.4527(35, C42H69O17: -Hex), 815.4423(20, C41H67O16), 以下18.69分の m/z 1007と共通				
20.09	1255.5939 (2.21E6)	C58H95O29	1123.5526(3.09E4; 100, C53H87O25: -Pen), 1093.5427(20, C52H85O24), 991.5108(15, C48H79O21: 1123-Pen), 977.4948(12, C47H77O21), 961.4997(20, C47H77O20), 以下 m/z 1417からの m/z 845以降と共通	20.16	686.3072 (2-, 3.22E5)		
20.34	1387.6360 (2.28E6)	C63H103O33	1255.5939(2.89E3; 100, C58H95O29: -Pen), 以下 m/z 1255と共通	20.39	722.3184 (2-, 6.23E6)	1385.6228 C63H101O33	1385→ 1295.5933(25, C60H95O30), 1253.5829(12, C5893O29), 843.4395(2.77E5; 100, C42H67O17), 541.1176(10, C21H33O16), 519.3328(12, C30H47O7), 469.1564(20, C18H29O14)
20.55	309.0875 (1.26E6)	C17H13O4N2	291.0761(8.15E5; 00, C17H11O3N2)				
20.58	1429.6324 (3.96E5)	C65H105O34		20.63	743.3238 (1.45E6)	1427.6354 C65H103O34	713.3140(2.69E5; 100, [M-2H]2-), 668.2973(2-, 20, C62H96O31), 647.2920(2-, 12, C60H94O30), 626.2871(2-, 3, (7, C58H92O29), 843.4393(20, C42H67O17), 583.1879(5, C23H35O17)
20.88	1371.6417 (5.95E5)	C63H103O32	1239.5999 (9.11E3; 100, C58H95O28: -Pen), 1107.5603(20, C53H87O24: 1239-Pen), 975.5186(15, C48H79O20: 1107-Pen), 945.5046(15, C47H77O19), 829.4572(12, C42H69O16), 813.4634(25, C42H69O15: 945-Pen), 783.4528(12, C41H67O14), 667.4052(20, C36H59O11), 651.4099(40, C36H59O10: 783-Pen), 487.3416(65, C30H47O5: 651-Hex(+2H)), 469.3309(25, C30H45O4)				

表1 キキョウのマススペクトルデータ(7)

21.48	1429.6460 (3.47E5)	C65H105O34		21.51	743.3238 (8.19E5)	1427.6354 C65H103O34	1427→ 1385.6263(55, C63H101O33), 1367.6157(7.36E4; 100, C63H99O32), 1337.6063(13, C62H97O31), 1295.5913(8, C60H95O30), 1277.5826(10, C60H93O29), 1253.5813(5, C58H93O29), 1235.5718(2, C58H91O28), 885.4501(7, C44H69O18), 843.4388(20, C42H67O17), 825.4290(10, C42H65O16), 795.4189(3, C41H63O15), 469.1573(2, C18H29O14)
22	1255.5939 (5.25E5)	C58H95O29		22.01	656.2967 (2-, 5.06E5)	1253.5817 C58H93O29	1253→ 1163.5497(15), 885.4493(8, C44H69O18), 843.4386(4.48E4; 100, C42H67O17), 825.4282(15, C42H65O16), 781.4388(15, C41H65O14), 681.3861(17, C36H57O12), 663.3751(15, C36H55O11), 519.3325(18, C30H47O7), 471.3116(7, C29H43O5)
				22.08	539.2604 (2-, 1.29E6)	1079.5286 C51H83O24	681.3857(10, C36H57O12), 509.2507(2-, 2.69E5; 100, C), 479.2400(2-, 50)
22.08	1239.5616 (1.06E6)	C57H91O29		22.14	1237.5499 (2.26E6)	C57H89O29	1219.5389(5, C57H87O28), 695.3660(3.26E5; 100, C36H55O13), 519.3331(15, C30H47O7)
22.14	1093.5411 (6.36E6)	C52H85O24	961.4994(40, C47H77O20: -Pen), 931.4893(15, C45H75O19), 829.4574(40, C42H69O16: 961-Pen), 815.4421(20, C41H67O16), 799.4470(45, C41H67O15), 683.3997(40, C36H59O12: 815-Pen), 667.4048(8.61E4; 100, C36H9O11), 以下18.69分のm/z 1417と共通	22.18	1091.5273 (4.27E6)	C52H83O24	1001.4971(5, C49H77O21), 723.3969(7, C38H59O13), 681.3865(5.72E5; 100, C36H57O12), 663.3759(10, C36H55O11), 519.3331(3, C30H47O7), 457.3325(3, C29H45O4)

表1 キキョウのマススペクトルデータ(8)

22.25	1387.6361 (1.31E6)	C63H103O33	1255.5939(2.89E3; 100, C58H95O29: -Pen), 以下 m/z 1255と共通	22.28	722.3179 (2-, 1.57E6)	1385.6226 C63H101O33	1385→ 1295.5933(25, C60H95O30), 1253.5811(30, C5893O29), 843.4386(1.02E5; 100, C42H67O17), 825.4275(15), 781.4379(15, C41H65O14), 681.3853(15, C36H57O12), 663.3748(17, C36H55O11), 541.1772(5,), 519.3325(18, C30H47O7), 471.3113(7, C29H43O5) 469.1561(10, C18H29O14)
22.39	1225.5839 (8.35E6)	C57H93O28 Platycodin B or D	1093.5422(1.31E4; 100), 以下22.14分の m/z 1093と共通	22.44	1223.5706 (1.22E7)	C57H91O28 Platycodin B or D	1205.5601(5, C57H89O27), 1133.5388(40, C54H85O25), 1091.5286(10, C52H83O24), 1073.5166(7, C51H81O23), 753.4063(10, C39H61O14), 723.3957(5, C38H59O13), 681.3860(1.10E6; 100, C36H57O12), 663.3754(3, C36H65O11), 541.1773(12, C21H33O16), 519.3322(3, C30H47O7), 469.1564(40, C18H29O14), 409.1349(3, C16H25O12)
				22.47	743.3238 (8.19E5)	1427.6354 C65H103O34	713.3139(5.44E5; 100, [M-2H]2-), 668.2977(2-, 20, C62H96O31)
22.58	1413.6516 (6.70E5)	C65H105O33		22.63	735.3265 (2-, 1.50E6)	1411.6416 C65H103O33	
	1267.5940 (4.71E6)	C59H95O29 Platycodin A or C	1135.5529(70, C54H87O25: -Pen), 1117.5416(15, C54H85O24), 1003.5105(25, C49H79O21), 871.4677(12, C44H71O17: 1003-Pen), 853.4578(25, C44H69O16), 823.4479(35, C43H67O15), 709.4155(22,), 691.4049(1.40E4; 100), 683.3997(30), 653.3894(25), 521.3469, 以下18.69分の m/z 1417と共通		662.2977 (9.18E6)	1265.5813 C59H93O29 Platycodin A or C	1265→ 1223.5712(80, C57H91O28), 1205.5616(5.19E5; 100, C57H89O27), 1175.5499(15, C56H87O26), 1133.5388(10, C54H85O25), 1115.5288(15, C54H83O24), 723.3962(20, C38H59O13), 681.3856(20, C36H57O12), 663.3749(10, C36H65O11), 541.1774(5, C21H33O16), 469.1563(15, C18H29O14),

表1 キキョウのマススペクトルデータ(9)

22.66	1209.5885 (2.65E6)	C57H93O27		22.69	1207.5752 (2.99E6)	C57H91O27	1117.5457(45, C47H89O29), 737.4128(12, C39H61O13), 707.4021(7, C38H59O12), 665.3922(2.60E5; 100, C36H57I1), 541.1782(10, C21H33O16), 469.1572(30, C18H29O14)
22.85	1239.5624 (3.75E5)	C57H91O29		22.89	1237.5498 (4.56E6)	C57H89O29	1207.5419(80,), 1027.4775(4.72E5; 100, C50H75O22), 695.3657(5, C36H55O13), 665.3548(5, C35H53O12), 541.1779(4, C21H33O16), 485.2912(7, C29H41O6), 469.1566(4, C18H29O14)
	1107.5210 (3.43E6)	C52H83O25					
22.89	1251.5883 (1.36E6)	C59H95O28		22.92	1249.5861 (1.37E6)	C59H93O28	1207.5769(1.56E5; 100, C57H91O27), 1189.5665(60, C57H89O26), 1159.5560(30, C56H87O25), 1117.5449(18, C54H85O24), 1099.5339(25, C54H83O23), 1057.5243(8, C52H81O22), 779.4237(5, C41H63O14), 737.4128(5, C39H61O13), 707.4024(50, C38H59O12), 665.3918(50, C36H57O11), 647.3812(20, C36H55O10), 469.1571(20, C18H29O14)
22.97	1149.5311 (2.45E6)	C54H85O26		22.85	1147.5188 (3.47E5)	C54H83O26	
				23.02	1279.5609 (2.23E6)	C59H91O30	1249.5531(70), 1069.4883(5.73E5; 100, C45H81O28), 1027.4773(10, C43H79O27), 665.3549(3, C35H53O12), 485.2916(5, C29H41O6: 665-Glc(+OH))

表1 キキョウのマススペクトルデータ(10)

23.12	1135.5518 (3.96E6)	C54H87O25		23.16	1133.5380 (6.02E5)	C54H85O25	1091.5292(80, C52H83O24), 1073.5182(20, C52H81O23), 1043.5066(7, C51H79O22), 983.4850(3, C49H75O20), 753.4081(5, C39H61O14), 723.3969(8.64E4; 100, C38H59O13), 681.3860(70, C36H57O12), 663.3757(25, C36H55O11), 633.3644(5, C35H53O10), 501.3229(2, C30H45O6: 663-Glc), 457.3331(2, C29H45O4)
23.2	1429.6466 (7.85E5)	C65H105O34		23.25	743.3238 (1.13E6)	1427.6354 C65H103O34	1427→ 1385.6254(75, C63H101O33), 1367.6160(1.65E5; 100, C63H99O32), 1337.6051(7, C62H97O31), 1295.5934(10, C60H95O30), 1277.5836(5, C60H93O29), 1253.5826(7, C58H93O29), 1205.5619(2, C50H93O32), 885.4498(7, C44H69O18), 843.4393(20, C42H67O17), 825.4288(10, C42H65O16), 519.3332(2, C30H47O7), 469.1573(2, C18H29O14)
23.42	1413.6512 (6.70E5)	C65H105O33		23.47	1411.6407 (6.81E5)	C65H103O33	
	1267.5935 (3.20E6)	C59H95O29 Platycodin A or C			1265.5823 (4.92E6)	C59H93O29 Platycodin A or C	1223.5719(80, C57H91O28), 1205.5620(1.79E5; 100, C57H89O27), 1175.5507(15, C56H87O26), 1133.5402(12, C54H85O25), 1115.5297(15, C54H83O24), 723.3972(20, C38H59O13), 681.3865(22, C36H57O12), 663.3761(10, C36H65O11), 541.1784(5, C21H33O16), 469.1569(15, C18H29O14)

表1 キキョウのマススペクトルデータ(11)

23.71	1251.5884 (1.61E6)	C55H95O31		23.78	1249.5850 (2.13E6)	C59H93O28	1207.5750(6.25E4; 100, C57H91O27), 1189.5645(60, C57H89O26), 1159.5541(30, C56H87O25), 1117.5438(18, C54H85O24), 1099.5333(25, C54H83O23), 1057.5217(8, C52H81O22), 779.4225(5, C41H63O14), 737.4114(10, C39H61O13), 707.4006(50, C38H59O12), 665.3903(45, C36H57O11), 647.3796(15, C36H55O10), 469.1562(20, C18H29O14)
23.83	1149.5308 (2.96E6)	C54H85O26		23.58	1147.5167 (3.68E5)		
				23.9	1279.5609 (3.04E6)	C59H91O30	1249.5518(85), 1069.4874(3.25E5; 100, C45H81O28), 1027.4764(10, C43H79O27), 665.3551(3, C35H53O12), 485.2912(5, C29H41O6: 665-Glc(+OH))
24.82	697.3765 (1.13R6)	C36H57O13					
24.92	683.3978 (9.59E6)	C36H59O12	521.3475(70, C30H49O7), 503.3369(90, C30H47O6), 485.3264(3.92E5; 100, C30H45O5), 455.3158(40, C29H43O4)				
25.49	697.3765 (2.73R6)	C36H57O13	535.3268(35, C30H47O8), 517.3165(7.40E5; 100, C30H45O7), 499.3058(10, C30H43O6), 455.3157(8, C29H43O4)				
25.64	667.4025 (6.42E5)	C36H59O11	505.3526(10, C30H49O6: -Hex), 487.3420(2.06E5; 100, C30H47O5), 469.3315(25, C30H45O4), 451.3209(10, C30H43O3)				

タイソウ

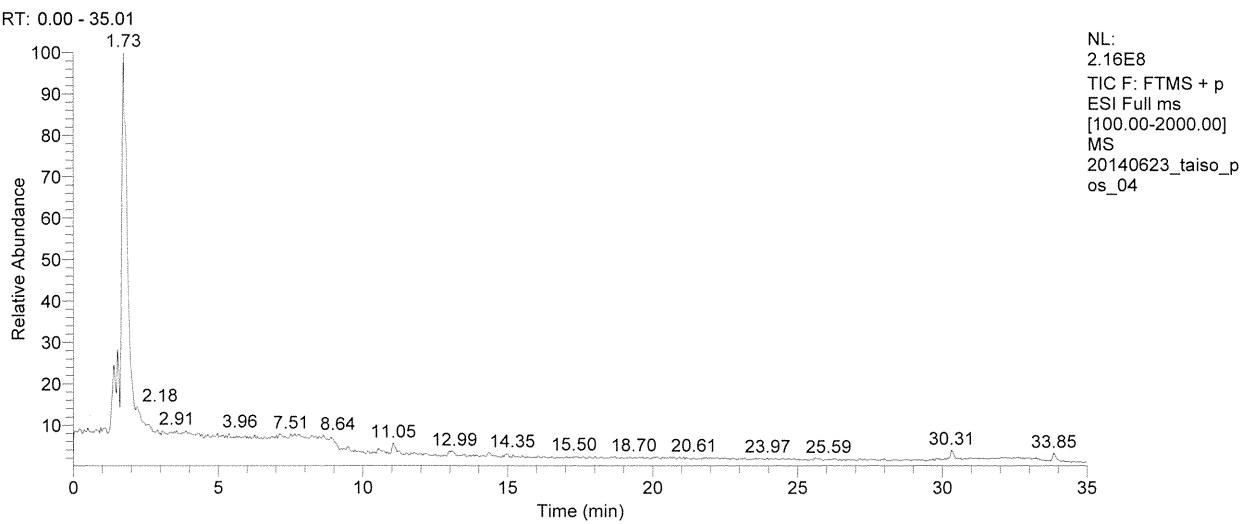


図 10 タイソウのポジティブモードにおける全イオンクロマトグラム(TIC)

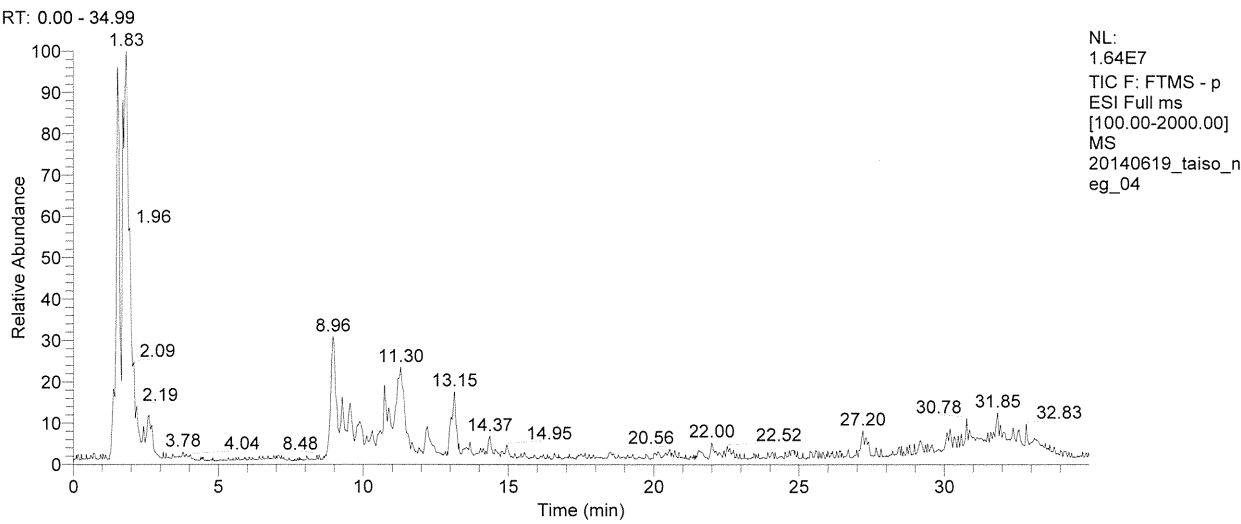


図 11 タイソウのネガティブモードにおける全イオンクロマトグラム(TIC)

20140619_Taiso_Neg_04 #575 RT: 13.07 AV: 1 NL: 4.74E5
T: FTMS - p ESI Full ms [100.00-2000.00]

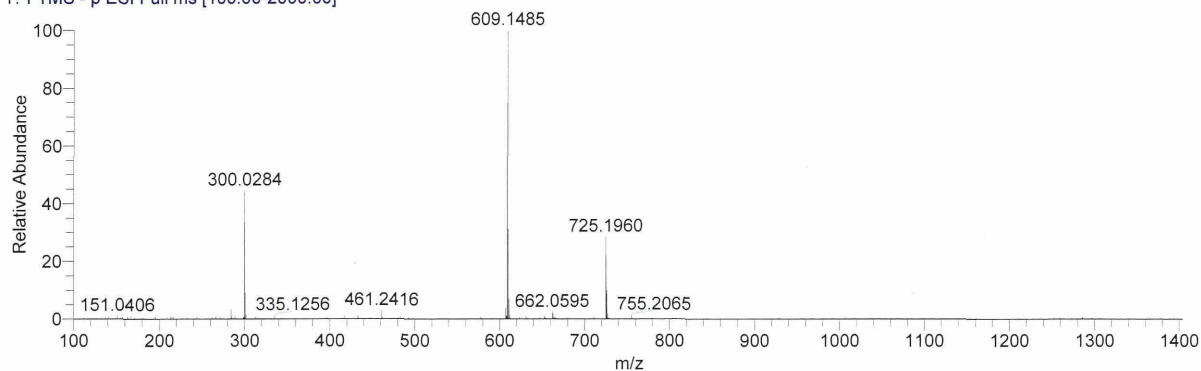


図 12 保持時間 13.07 分のピークのマススペクトル

20140619_Taiso_Neg_04 #582 RT: 13.22 AV: 1 NL: 6.99E4
T: FTMS - p ESI d Full ms2 609.15@cid35.00 [155.00-620.00]

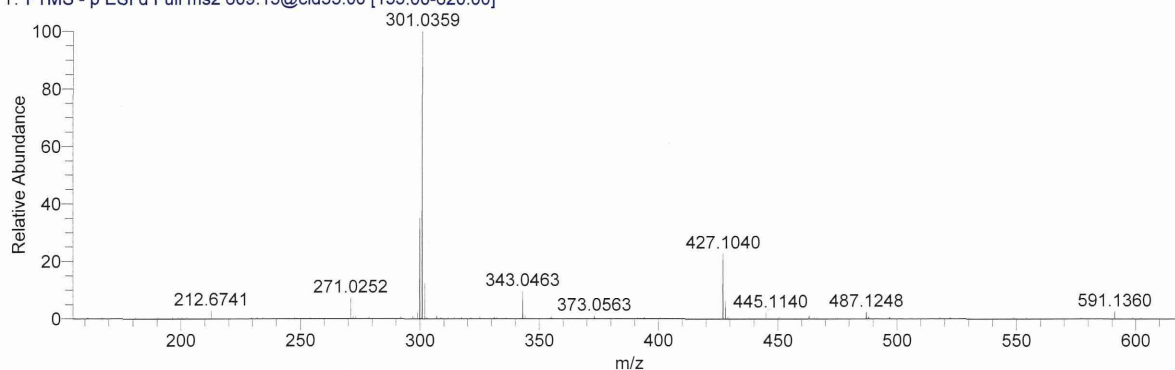


図 13 m/z 609 をプリカーサーイオンとした MS/MS

20140619_Taiso_Neg_04 #572 RT: 12.99 AV: 1 NL: 1.91E4
T: FTMS - p ESI d Full ms2 725.20@cid35.00 [185.00-740.00]

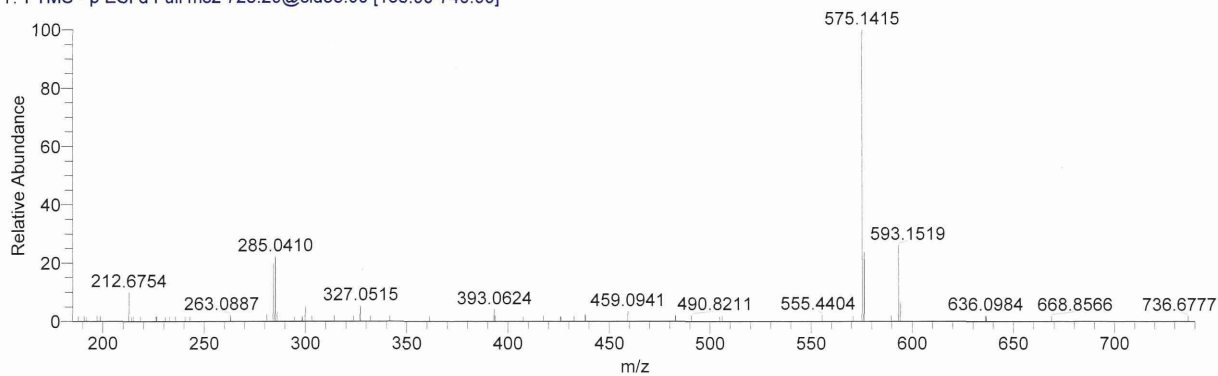


図 14 m/z 725 をプリカーサーイオンとした MS/MS

20140619_Taiso_Neg_04 #928 RT: 21.26 AV: 1 NL: 4.42E4
T: FTMS - p ESI Full ms [100.00-2000.00]

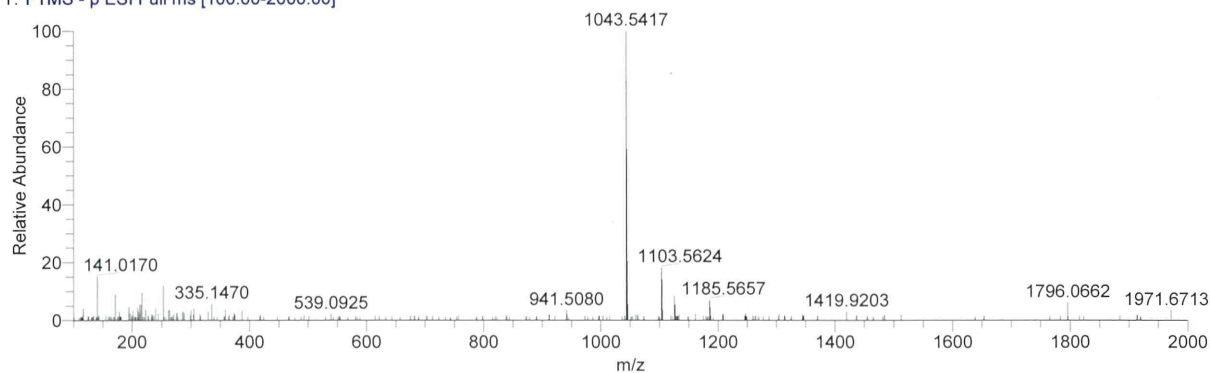


図 15 保持時間 21.54 分のピークのマススペクトル

20140619_Taiso_Neg_04 #927 RT: 21.23 AV: 1 NL: 3.51E4
T: FTMS - p ESI d Full ms2 1043.54@cid35.00 [275.00-1055.00]

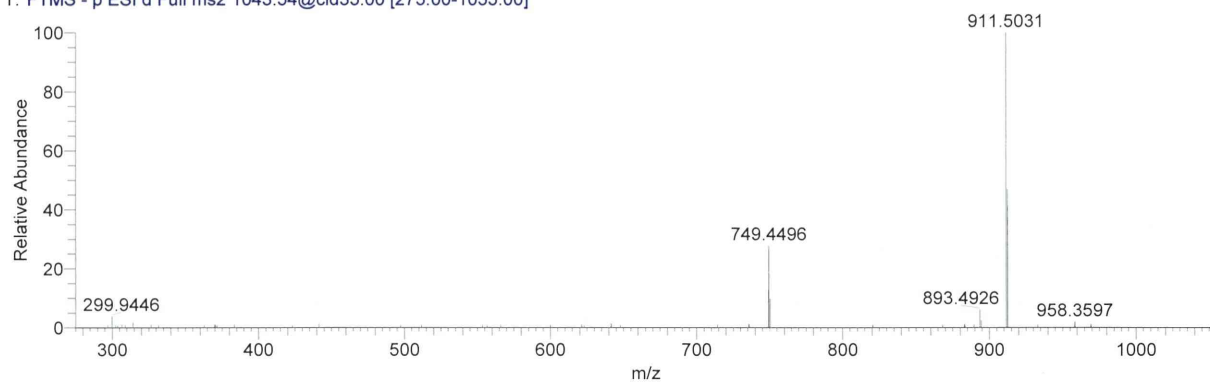


図 16 m/z 1043 をプリカーサーイオンとした MS/MS

表2 タイソウのマススペクトルデータ(1)

Positive				Negative			
r.t.	m/z	Fomula	Product Ions	r.t.	m/z	Fomula	Product Ions
1.38	203.0405 (2.75E6)		179.0400(15), 161.0295(1.66E6; 100), 143.0189(70)	1.39	201.0261 (1.88E5)		
					359.0156 (2.24E5)		217.0030(2.01E5; 100), 201.0255(7)
	184.0459 (4.97E6)		179.0400(15), 161.0295(5.61E5; 100), 143.0188(80), 124.0244(25)				
	161.0299		161(1.61E6; 100), 143.0190(85)				
1.53	316.9208 (2.93E6)		234.9174(50), 218.9435(9.44E5), 136.9402(10)				
	398.9237 (1.42E6)		316.9210(75), 300.9470(3.66E5; 100), 234.9174(15), 218.9434(20)				
1.73	176.0921 (2.28E7)	C7H14O4N	158.0810(70, C7H12O3N), 140.0704(60, C7H10O2N), 130.0861(7.75E6; 100, C6H12O2N), 128.0706(15, C6H10O2N)	1.71	174.0777 (2.43E6)	C7H12O4N	174(3.26E5; 100), 156.0669(35, C7H10O3N), 138.0562(20, C7H8O2N), 129.0197(45, C5H5O4), 124.0406(20, C6H6O2N), 102.0564(25, C4H8O2N), 85.0299(10, C4H5O2)
					293.0998 (1.69E6)		275.0886(15), 245.0784(50), 203.0678(8.09E4; 100), 131.0466(35)
	325.1135 (2.66E7)	C12H21O10	307.1030(15, C12H19O9), 289.0923(85, C12H17O8), 271.0817(2.51E6; 100, C12H15O7), 253.0710(65, C12H13O6), 241.0708(15, C11H13O6), 223.0602(40, C11H11O5), 163.0600(25, C6H11O5), 145.0495(45, C6H9O4), 127.0390(25, C6H7O3)				
1.78	160.0972 (3.48E7)	C7H14O3N	142.0859(10, C7H12O2N), 114.0912(4.52E6; 100, C6H12ON)				
1.81	278.1237 (2.30E7)	C11H20O7N	260.1131(2.19E7; 100, C11H18O6N), 242.1024(2, C11H16O5N), 212.0553(2, C9H10O5N)				

表2 タイソウのマススペクトルデータ(2)

	260.1132	C11H16O5N	242.1026(2.40E7; 100, C11H16O5N), 232.1182(25, C10H18O5N), 214.1075(5, C10H16O4N), 128.0706(3, C6H10O2N)				
				1.87	424.1101 (2.89E5)		364.0891(4.12E4; 100), 346.0784(55), 304.0676(25)
					439.0865 (5.94E5)		421.0750(80), 341.1090(4.99E3; 100), 277.0331(95)
				2	597.1083 (1.84E5)		579.0978(25), 499.1309(1.57E4; 100), 417.0443(35), 337.0777(60), 259.0227(55)
				8.96	638.1822 (2-, 3.28E5)		1101.3383(10), 951.2847(25), 647.2049(25), 608.1711(2-, 1.01E5; 100), 572.1603(2-, 15), 550.1657(2-, 60), 520.1549(2-, 45), 484.1440(2-, 10)
				9.05	645.1902 (2-, 9.00E4)		965.2989(25), 615.1780(2-, 1.95E4; 100), 579.1681(2-, 15), 550.1655(2-, 10), 527.1616(2-, 20)
					575.2210 (6.88E4)	C22H39O17	413.1664(1.52E4; 100, C16H29O12: -Glc)
				9.23	673.2207 (9.10E4)	C26H41O20	655.2093(7.59E3; 100, C26H39O19), 435.1508(30, C18H27O12)
					923.3266 (6.77E4)	C36H59O27	905.3154(5.40E3; 100, C36H57O26), 805.2991(60, C32H53O23), 483.1727(75, C19H31O14)
				9.28	645.1900 (2-, 1.77E5)		965.2996(15), 615.1780(2-, 4.27E4; 100), 579.1677(2-, 15), 510.1411(2-, 10), 480.1302(2-, 10)
					1291.3879 (1.63E5)		1273.3750(5), 1231.3645(25), 1115.3540(1.76E5; 100), 1055.3325(30), 983.3106(5)
9.46	448.1964 (1.71E6)	C23H30O8N	431.1710(3, C23H27O8), 286.1439(3.25E5; 100, C17H20O3N: -Glc), 269.1173(85, C17H17O3), 237.0909(5, C16H13O2), 209.0959(2, C15H13O), 175.0752(3, C11H11O2)				
10.54	286.1438 (1.79E6)	C17H20O3N	269.1174(1.62E6; 100, C17H17O3), 237.0909(5, C16H13O2), 175.0752(7, C11H11O2)				

表2 タイソウのマススペクトルデータ(3)

				9.55	1097.3818 (4.08E5)	C43H69O32	1079.3690(50), 979.3527(55), 937.3418(60), 919.3316(5.22E4; 100), 773.2729(15), 659.2409(10), 615.2151(40)
					965.3392	C38H61O28 1097-Pen	947.3260(2.08E4; 100, C38H59O27), 847.3095(15, C34H55O24), 805.2996(35, C32H53O23), 787.2888(45, C32H51O22), 727.2679(20, C30H47O20), 659.2415(15, C26H43O19), 525.1829(10, C21H33O15), 483.1725(70, C19H31O14)
				9.75	951.3237 (4.53E4)		
				9.84	1243.4409 (2.34E5)		1183.4172(1.48E5; 100), 1111.3948(15), 965.3365(20, C38H61O28)
				9.89	1375.4821 (1.20E5)		1315.4622(1.53E5; 100), 1243.4392(20), 1097.3793(15, C43H69O32)
				10.36	771.2009 (1.09E5)	C33H39O21	609.1462(1.75E5; 100, C27H29O16: -Glc)
				10.64	993.3322 (6.85E4)		933.3093(3.24E4; 100), 861.2878(12), 715.2308(35)
				10.69	755.2064 (8.08E4)	C33H39O20	593.1517(1.13E5; 100, C27H29O15: -Glc)
10.71	597.1795 (5.05E5)	C27H33O15	579.1722(15, C27H31O14), 561.1614(80, C27H29O13), 543.1507(25, C27H27O12), 525.1398(60, C27H25O11), 513.1397(8, C26H25O11), 477.1397(20, C23H25O11), 459.1291(1.81E5; 100, C23H23O10), 447.1080(7, C25H19O8)	10.74	595.1682 (6.76E5)	C27H31O15	577.1571(25, C27H29O14), 505.1362(45, C24H25O12), 487.1254(20, C24H23O11), 475.1255(95, C23H23O11), 457.1149(30, C23H21O10), 415.1043(35, C21H19O9: -Glc(+OH)), 385.0936(95, C20H17O8), 355.0830(6.59E4; 100, C19H15O7)
				10.92	593.2101 (3.91E5)	C25H37O16	431.1564(2.52E5; 100, C19H27O11: -Glc), 269.1036(5, C13H17O6: 431-Glc)

表2 タイソウのマススペクトルデータ(4)

					431.1568	C19H27O11	269.1036(3.44E4; 100, C13H17O6: -Glc), 161.0459(15, C6H9O5)
11.05	342.1705 (4.34E6)	C20H24O4N	311.1283(20, C19H19O4), 297.1128(2.20E6; 100, C18H17O4), 279.1019(13, C18H15O3), 265.0862(30, C17H13O3)				
				11.21	1285.4512 (4.78E5)	C51H81O37	1225.4283(3.58E5; 100, C49H77O35), 1153.4064(12, C46H73O33: -Pen), 1007.3482(15, C40H63O29: 1153-Glc(-O))
				11.3	1139.3927 (3.68E5)	C45H71O33	1121.3788(95, C45H69O32), 1079.3683(25, C43H67O31), 1021.3642(25, C41H65O29), 961.3419(85, C39H61O27), 919.3316(90, C37H59O26), 901.3209(1.41E4; 100, C37H57O25), 615.2151(60, C24H39O18)
					1417.4946 (2.27E5)	C56H89O41	1357.4708(2.53E5; 100, C54H85O39), 1297.4486(5, C52H81O37), 1285.4486(15, C51H81O37), 1225.4272(3, C49H77O35), 1139.3899(12, C45H71O33)
				11.4	1007.3499 (3.92E5)	C40H63O29	989.3367(1.57E4; 100, C40H61O28), 861.2899(15, C34H53O25), 847.3099(15, C34H55O24), 829.2999(20, C34H53O23), 787.2887(25, C32H51O22), 769.2786(30, C32H49O21), 727.2682(15, C30H47O20), 667.2471(12, C28H43O18), 483.1727(75, C19H31O14)
				11.73	711.3098 (5.83E4)	C31H51O18	549.2561(4.43E4; 100, C25H41O13: -Glc), 387.2027(8, C19H31O8)

表2 タイソウのマススペクトルデータ(5)

12.15	743.2000 (4.51E5)	C32H39O20	611.1633(45, C27H31O16), 597.1475(13, C26H29O16: -Glc(-O)), 465.1040(25, C21H21O12: 597-Pen), 449.1090(8, C21H21O11), 303.0504(1.84E5; 100, C15H11O7: 465-Glc)	12.17	741.1900 (4.59E5)	C32H37O20	723.1782(15, C32H35O19), 609.1466(50, C27H29O16: -Pen), 591.1362(2.26E4; 100, C27H27O15), 573.1255(15, C27H25O14), 475.0885(35, C22H19O12: 609-Pen(+2H)), 343.0461(15, C17H11O8: 475-Pen), 300.0279(95, C15H8O7), 271.0251(20, C14H7O6)
12.99	463.2545 (2.73E5)	C22H39O10	446.2296(50), 445.2455(95, C22H37O9), 435.2611(50, C21H39O9), 418.2346(5.34E4; 100,), 417.2505(95, C21H37O8), 399.2400(40, C21H35O7), 350.1715(30, C19H26O6), 336.1923(25, C19H28O5), 319.1657(50,), 223.1076(25), 206.0811(15, C8H14O6)				
	727.2054 (1.68E5)			13.02	725.1960 (1.81E5)	C32H37O19	593.1519(25, C27H29O15: -Pen), 575.1415(1.91E4; 100, C27H27O14), 285.0410(20, C15H9O6)
13.07	611.1591 (1.49E6)	C27H31O16	465.1036(40, C21H21O12), 449.1087(7, C21H21O11: -Glc), 303.0502(4.44E5; 100, C15H11O7)	13.15	609.1485 (1.15E6)	C27H29O16	591.1360(3, C27H27O15), 427.1040(25, C22H19O9), 343.0463(12, C17H11O8), 301.0359(6.99E4; 100, C15H9O7), 271.0252(10, C14H7O6)
	rutin			13.54	597.1843 (5.06E4)	C27H33O15	579.1719(13, C27H31O14), 507.1508(10, C24H27O12), 489.1399(15, C24H25O11), 477.1401(2.89E4; 100, C23H25O11), 459.1293(20, C23H23O10), 417.1187(30, C21H21O9: -Glc(+OH)), 387.1083(70, C20H19O8), 357.0979(75, C19H17O7)
13.6	595.1647 (1.03E5)	C27H31O15		13.68	593.1527 (1.42E5)	C27H29O15	327.0513(25, C17H11O7), 285.0411(1.51E4; 100, C15H9O6), 284.0331(60, C15H8O6)
14	595.1639 (1.28E5)	C27H31O15		14.04	593.1526 (1.27E5)	C27H29O15	285.0409(2.74E4; 100, C15H9O6)

表2 タイソウのマススペクトルデータ(6)

	639.3215 (1.71E5)	C29H51O15	621.3153(30, C29H49O14), 603.3043(3, C29H47O13), 585.2935(5, C29H45O12), 567.2829(10, C29H43O11), 555.2828(1.76E5; 100, C28H43O11), 477.2717(10, C23H41O10)				
14.27	581.1487 (1.69E5)	C26H29O15	449.1085(85, C21H21O11: -Pen), 431.0981(10, C21H19O10), 413.0873(7, C21H17O9), 345.0607(3, C17H13O8), 303.0500(1.00E5; 100, C15H11O7),	14.37	579.1371 (1.48E5)	C26H27O15	447.0933(15, C21H19O11), 429.0832(20, C21H17O10), 300.0279(1.94E4; 100, C15H8O7), 271.0251(15, C14H7O6)
14.35	477.2699 (1.64E6)	C23H41O10	460.2452(70), 459.2611(85, C23H39O9), 449.2769(60, C22H41O9), 432.2503(99), 431.2664(2.64E5; 100, C22H39O8), 413.2556(40, C22H37O7), 396.2292(8), 364.1873(35, C20H28O6), 336.1923(30, C19H28O5), 319.1657(60, C22H23O2), 227.1753(12, C17H23), 223.1076(25, C16H15O), 206.0810(15, C8H14O6)	14.37	475.2576 (1.69E5)	C23H39O10 (?)	458.2297(25), 431.2666(45, C22H39O8), 414.2400(20,), 266.1150(4.59E4; 100, C14H18O5), 249.0883(15, C17H13O2(?))
14.57	673.3064 (1.49E5)	C32H49O15	655.3007(30, C32H47O14), 637.2897(2, C32H45O13), 619.2791(5, C32H43O12), 601.2679(10, C32H41O11), 589.2682(1.40E5; 100, C31H41O11), 511.2568(10, C26H39O10: -Glc)				
				14.85	783.2156 (5.90E4)	C38H39O18	663.1720(98, C34H31O14), 607.1671(5.83E3; 100, C28H31O15), 427.1038(85, C22H19O9)

表2 タイソウのマススペクトルデータ(7)

14.97	511.2544 (1.25E6)	C26H39O10	494.2303(85), 493.2461(80, C26H37O9), 483.2617(65, C25H39O9), 466.2352(2.13E5; 100,), 465.2513(99, C25H37O8), 447.2406(40, C25H35O7), 430.2140(7, C21H34O9), 380.1614(5, C23H24O5), 370.1771(30, C22H26O5), 364.1876(20, C20H28O6), 353.1505(55,), 318.1819(15, C19H26O4), 261.1601(15, C20H21), 233.1650(7), 223.1078(15, C16H15O)	14.95	509.2422 (1.81E5)	C26H37O10 (?)	492.2137(40), 465.2506(70, C25H37O8), 448.2240(30,), 344.1614(20, C20H24O5), 266.1149(2.26E4; 100, C14H18O5), 249.0883(15, C17H13O2(?))
					531.2240 (6.58E4)	C25H31O10 (?)	514.1962(35,), 504.2114(30), 487.2329(40), 476.2167(9.16E3; 100), 469.2220(50), 346.1058(25)
15.46	535.2751 (1.02E5)	C25H43O12					
16.08	569.2593 (8.75E4)	C28H41O12					
				17.51	935.4333 (7.93E4)	C40H71O24	917.4240(40, C40H69O23), 773.3818(1.72E4; 100, C34H61O19: -Glc), 755.3713(30, C34H59O18), 611.3284(10, C28H51O14: 773-Glc)
18.61	219.1745 (3.33E5)	C15H23O	203.1431(3.65E5; 100, C14H19O)				
				18.93	773.3802 (3.84E4)	C34H61O19	755.3716(50, C34H59O18), 611.3294(1.41E4; 100, C28H51O14: -Glc), 593.3193(25, C28H49O13),
				20.15	517.3173 (4.78E4)	C30H45O7	487.3069(4.49E4; 100, C29H43O6), 455.3162(7, C29H43O4)
					531.2966 (9.87E4)	C30H43O8	513.2863(20, C30H41O7), 501.2855(7.42E3; 100, C29H41O7), 487.3063(85, C29H43O6), 469.2953(35, C29H41O5)
				20.56	329.2332 (6.16E4)	C18H33O5	311.2228(45, C18H31O4), 229.1447(80, C12H21O4)
				21.26	1043.5417 (1.35E5)	C52H83O21 Zizyphus saponin III	911.5031(3.51E4; 100, C47H75O17: -Pen), 893.4926(10, C47H73O16), 749.4496(30, C41H65O12: 911-Glc)

表2 タイソウのマススペクトルデータ(8)

				21.54	1043.5427 (1.35E5)	C52H83O21 Zizyphus saponin III	911.5021(9.44E4; 100, C47H75O17: -Pen), 893.4902(10, C47H73O16), 749.4483(25, C41H65O12: 911-Glc)
				21.69	911.5000 (7.83E4)	C47H75O17 Zizyphus saponin I or II	765.4432(3), 749.4493(8.49E4; 100, C41H65O12: -Glc), 603.3907(10, C35H55O8: 749-Glc(-O))
				22	911.5000 (2.39E5)	C47H75O17 Zizyphus saponin I or II	765.4443(2), 749.4496(3.30E4; 100, C41H65O12: -Glc), 603.3907(10, C35H55O8: 749-Glc(-O))
				22.25	501.3222 (7.56E4)	C30H45O6	439.3224(2.48E4; 100, C29H43O)
				22.52	515.3020 (1.54E5)	C30H43O7	497.2913(25, C30H41O6), 471.3123(3.21E4; 100, C29H43O5), 453.3016(25, C29H41O4), 409.3116(12, C28H41O2)
				22.67	911.5006 (5.17E4)	C47H75O17 Zizyphus saponin I or II	765.4438(12), 749.4497(4.35E4; 100, C41H65O12: -Glc), 603.3914(10, C35H55O8: 749-Glc(-O))
				24.39	501.3228 (5.69E4)	C30H45O6	471.3123(4.44E4; 100, C29H43O5), 439.3223(12, C29H43O3)
				24.66	529.3173 (6.34E4)	C31H45O7	485.3271(1.16E4; 100, C30H45O5)
				24.83	487.3428 (8.91E4)	C30H47O5	469.3322(2.30E4; 100, C30H45O4),
25.59	383.1676 (1.92E5)		300.1638(25), 253.1048(7.45E3; 100)				
25.63	555.3163 (3.04E5)	C29H47O10	456.2385(5.17E4; 100, C23H36O9)				
27.16	487.3409 (1.43E5)	C30H47O5	469.3319(15, C30H45O4), 451.3210(8, C30H43O3), 441.3368(8.84E4; 100, C29H45O3), 423.3261(20, C29H43O2), 405.3153(8, C29H41O), 237.1482(10, C14H21O3)	27.2	485.3289 (3.94E5)	C30H45O5	439.3211(3, C29H43O3), 423.3272(4.79E4; 100, C29H43O2)

表2 タイソウのマススペクトルデータ(9)

27.3	503.3359 (6.68E4)	C30H47O6		27.3	501.3223 (1.72E5)	C30H45O6	471.3123(1.20E5; 100, C29H43O5), 453.3011(3, C29H41O4), 439.3223(5, C29H43O3), 425.3062(12, 28H41O3), 409.3112(7, C28H41O2)
	485.3253 (8.40E4)	C30H45O5					
27.91	251.2006 (2.02E5)	C16H27O2	233.1899(2.31E4; 100, C16H25O), 215.1793(95, C16H23), 205.1949(25, C15H25), 195.1378(25, C12H19O2), 181.1222(20, C11H17O2), 167.1429(15, C11H19O)				
				29.17	471.3493 (3.37E5)	C30H47O4	
					553.3524 (5.40E4)	C34H49O6	471.3489(4.76E4; 100, C30H47O4)
				29.58	471.3493 (1.60E5)	C30H47O4	423.3267(65, C29H43O2)
					553.3524 (3.34E4)	C34H49O6	471.3484(7.25E4; 100, C30H47O4)
				30.05	469.3334 (1.45E5)	C30H45O4	
					551.3365 (5.10E4)	C34H47O6	469.3329(5.10E4; 100, C30H45O4)
30.18	487.3410 (1.53E5)	C30H47O5		30.2	485.3286 (4.43E5)	C30H45O5	467.3167(2, C30H43O4), 439.3215(5, C29H43O3), 423.3268(1.85E5; 100, C29H43O2)
				30.78	453.3023 (1.69E5)	C29H41O4	409.3113(1.09E5; 100, C28H41O2),
				30.88	617.3863 (2.96E5)	C39H53O6	497.3277(2.14E4; 100, C31H45O5), 453.3379(55, C30H45O3)
				31.8	455.3541 (5.04E5)	C30H47O3 Oleanolic acid or Betulinic acid	