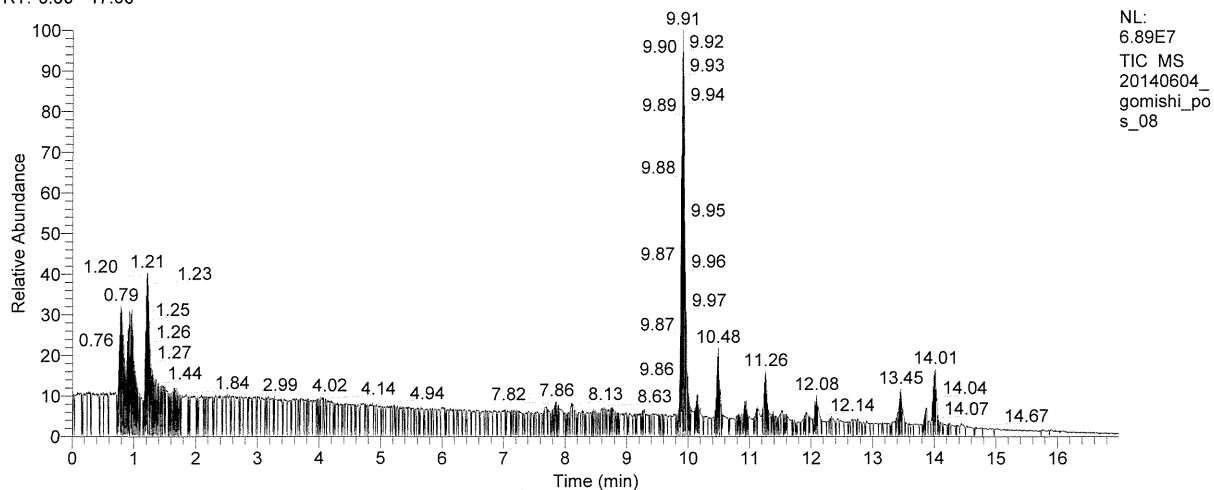


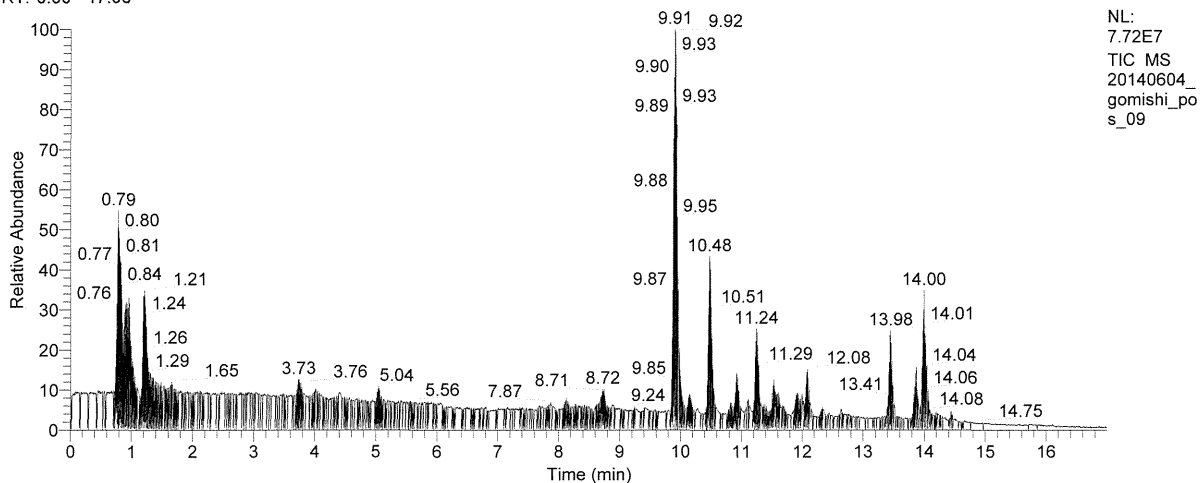
NIB-357

RT: 0.00 - 17.00



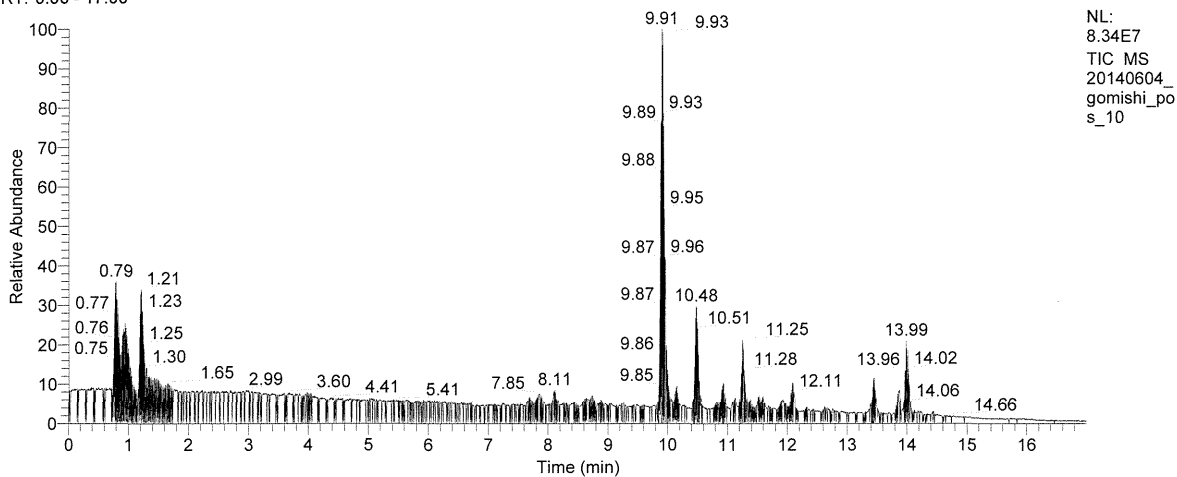
NIB-358

RT: 0.00 - 17.00

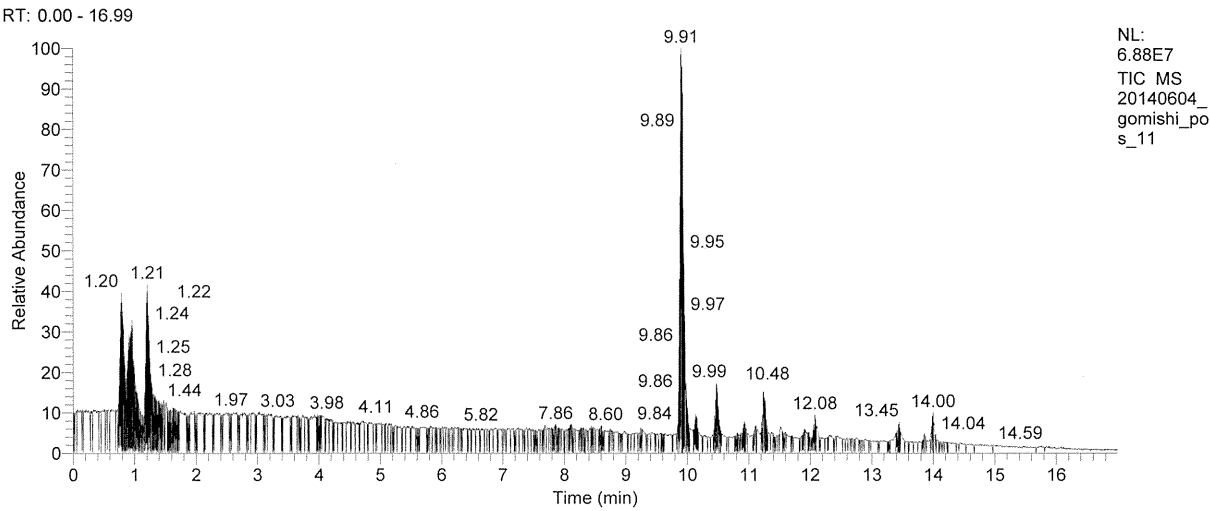


NIB-359

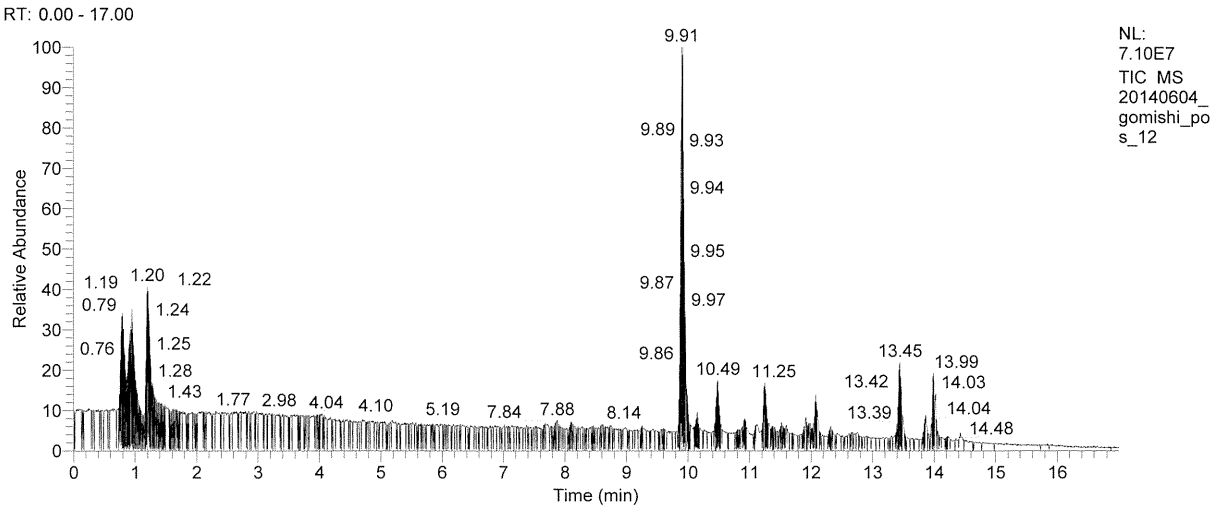
RT: 0.00 - 17.00



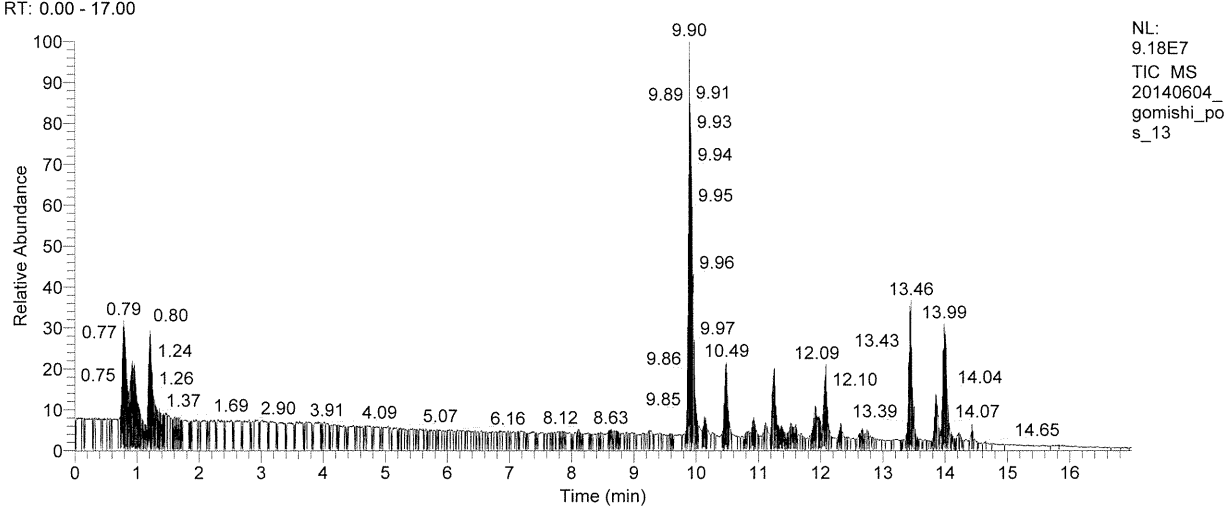
NIB-360



NIB-437

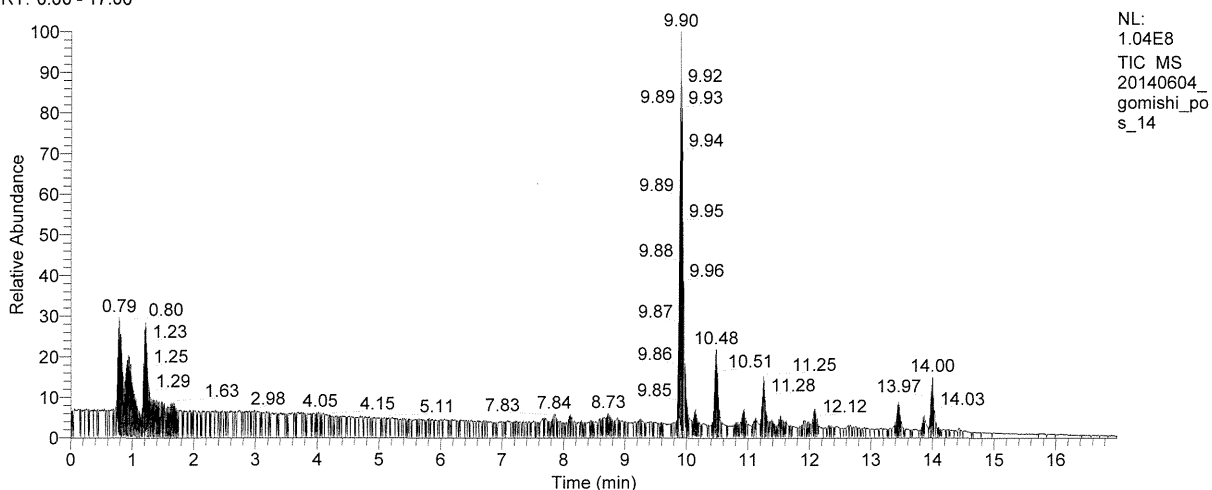


NIB-446



NIB-646

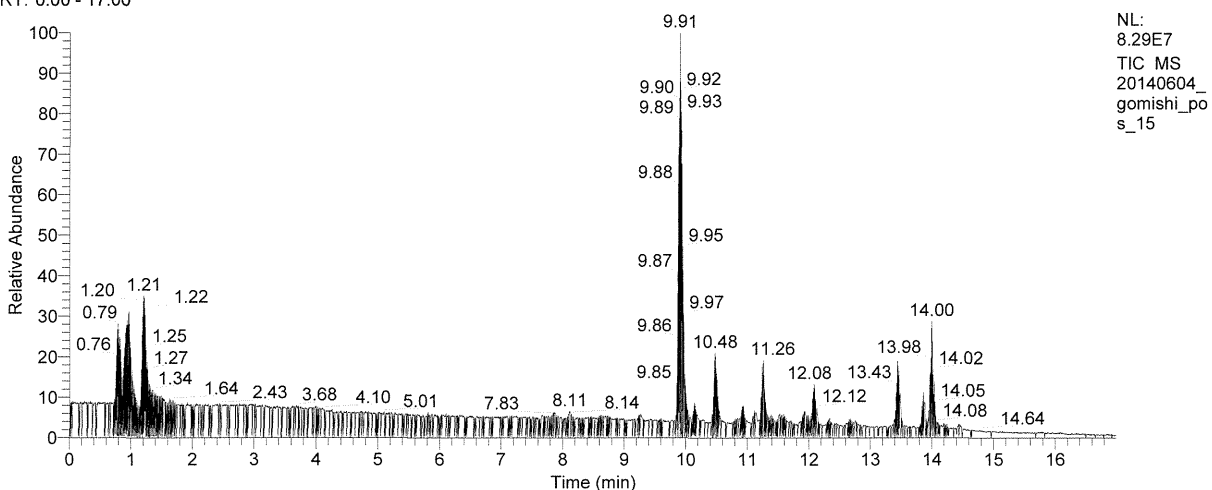
RT: 0.00 - 17.00



NL:
1.04E8
TIC MS
20140604_
gomishi_po
s_14

NIB-737

RT: 0.00 - 17.00



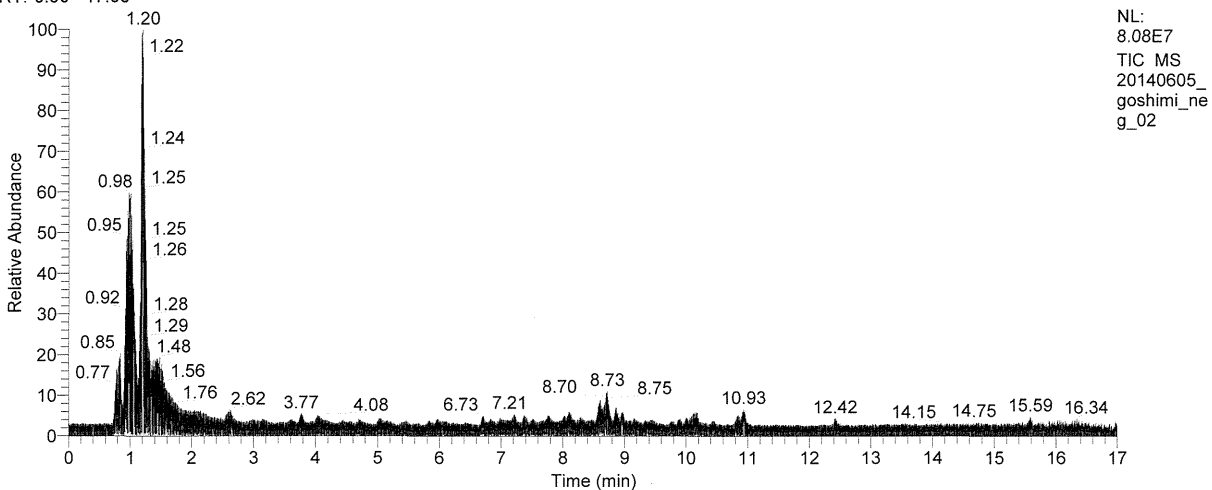
NL:
8.29E7
TIC MS
20140604_
gomishi_po
s_15

ゴミシ LC/MS データ (negative mode)

TIC

NIB-246

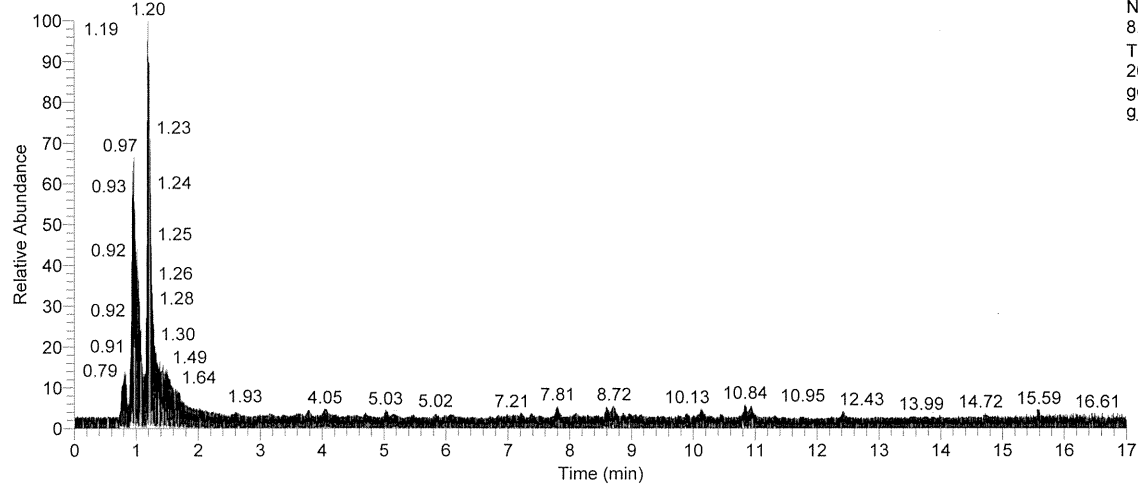
RT: 0.00 - 17.00



NL:
8.08E7
TIC MS
20140605_
goshimi_ne
g_02

NIB-270

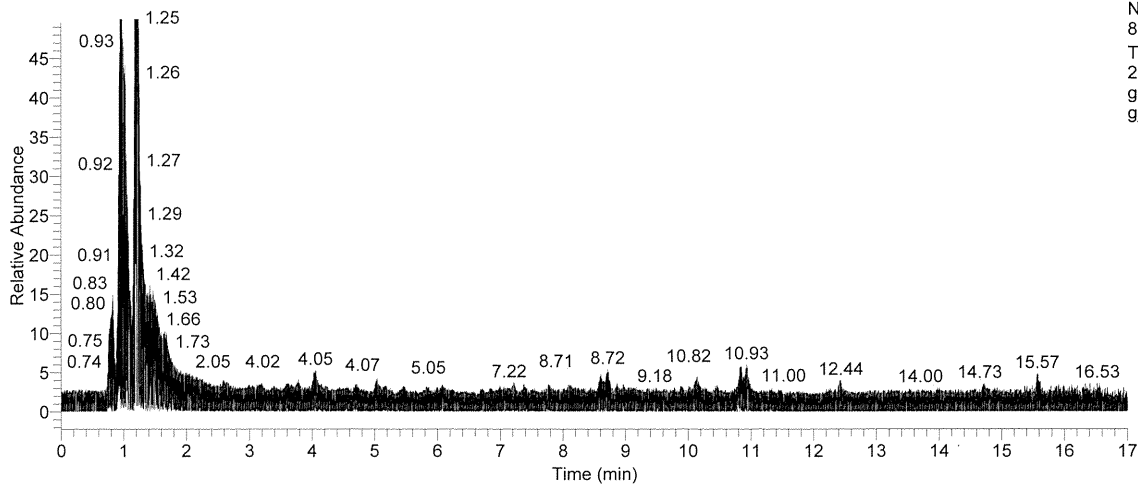
RT: 0.00 - 17.00



NL:
8.39E7
TIC MS
20140605_
goshimi_ne
g_03

NIB-353

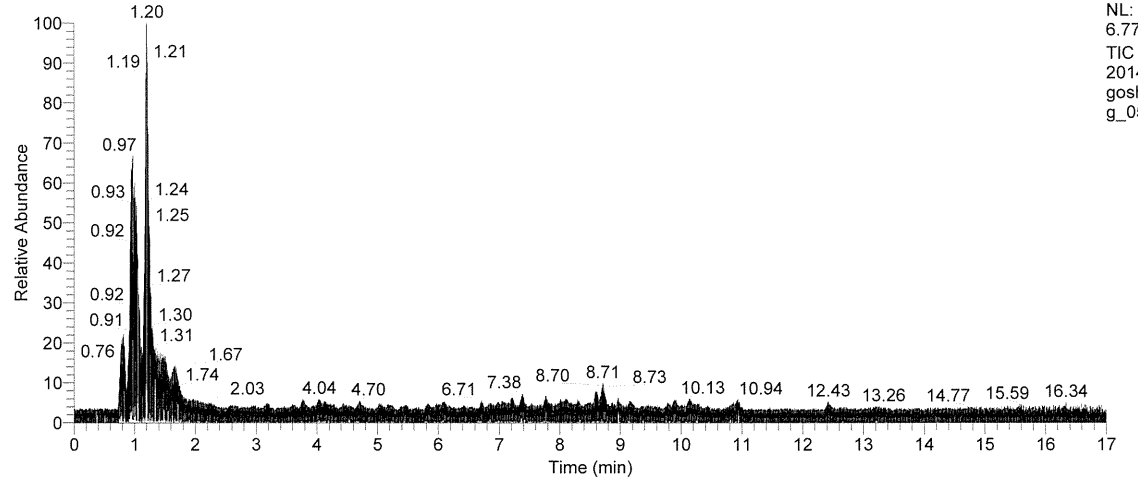
RT: 0.00 - 17.01



NL:
8.76E7
TIC MS
20140605_
goshimi_ne
g_04

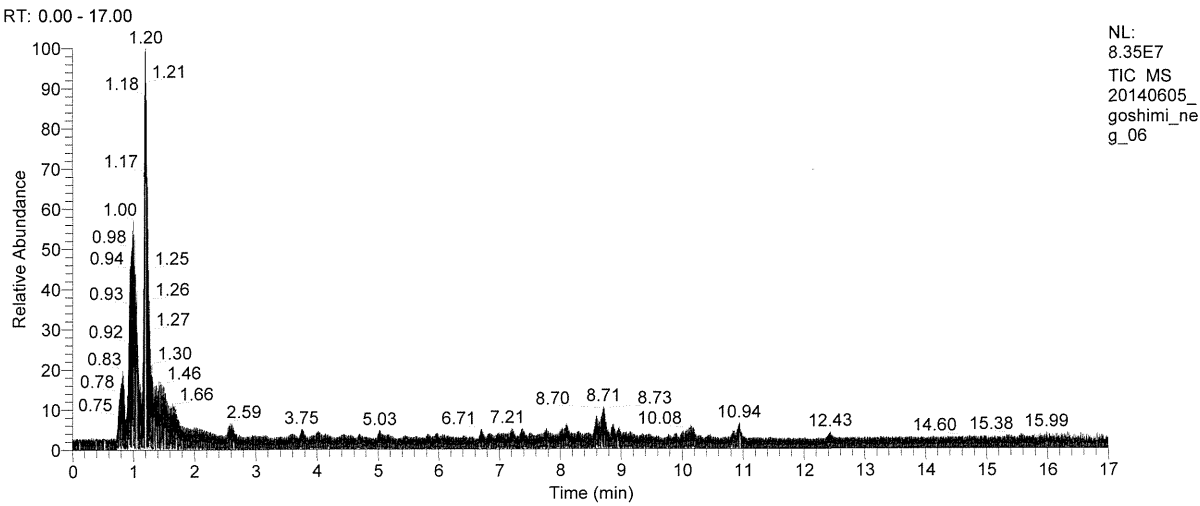
NIB-354

RT: 0.00 - 17.00

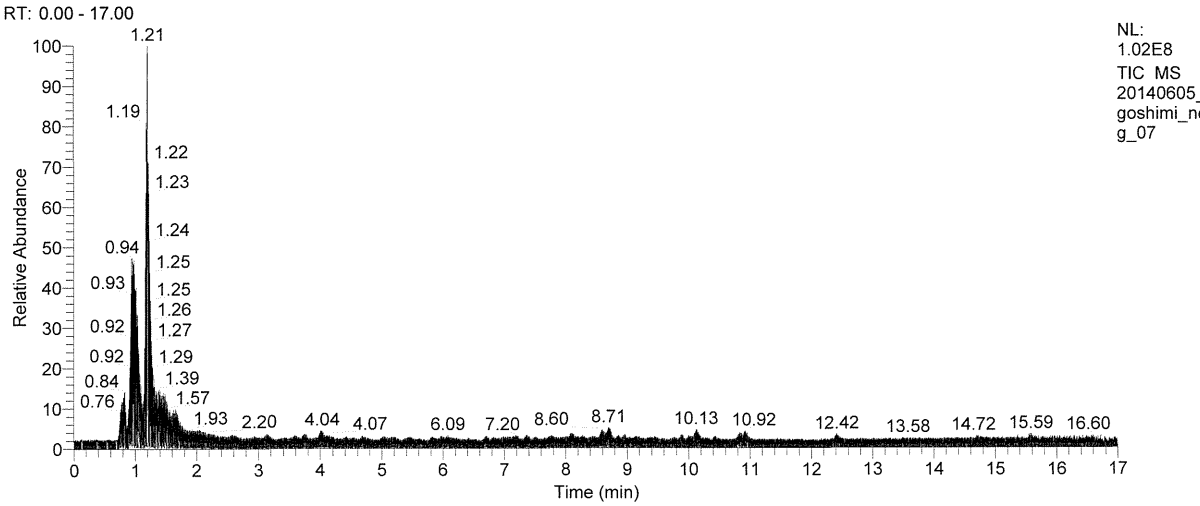


NL:
6.77E7
TIC MS
20140605_
goshimi_ne
g_05

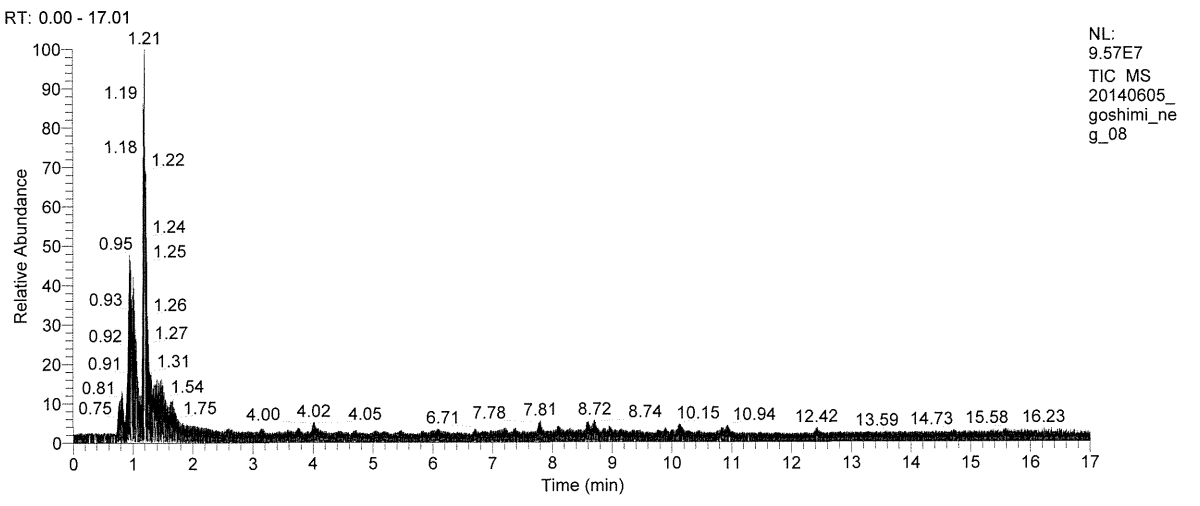
NIB-355



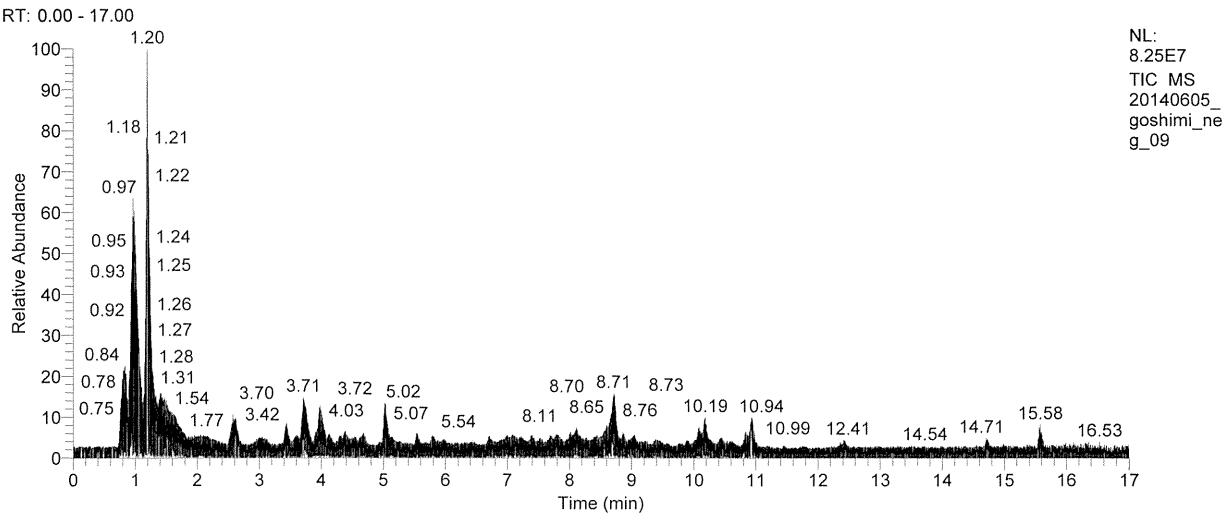
NIB-356



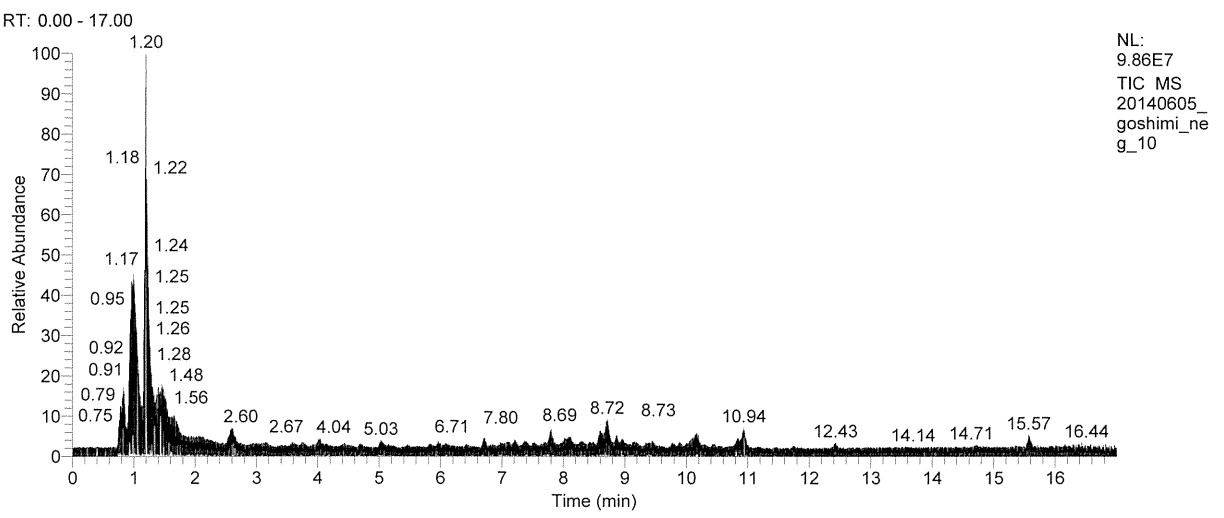
NIB-357



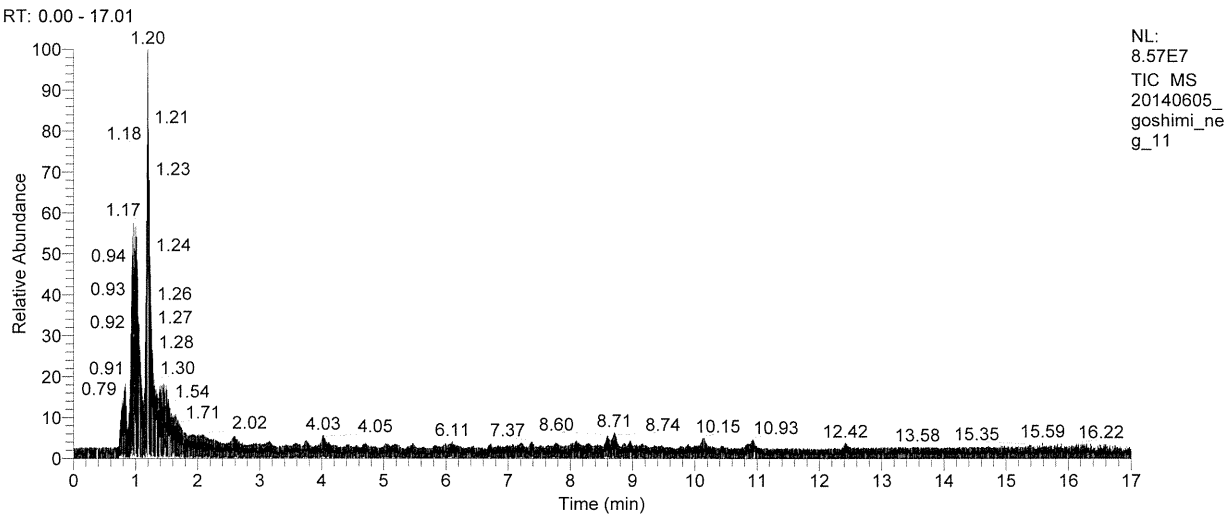
NIB-358



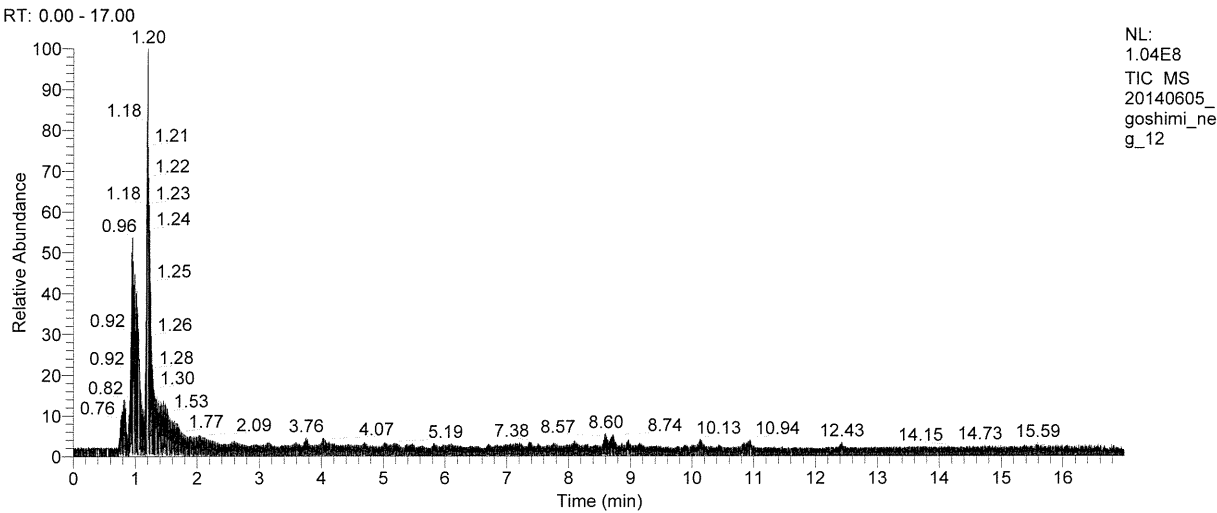
NIB-359



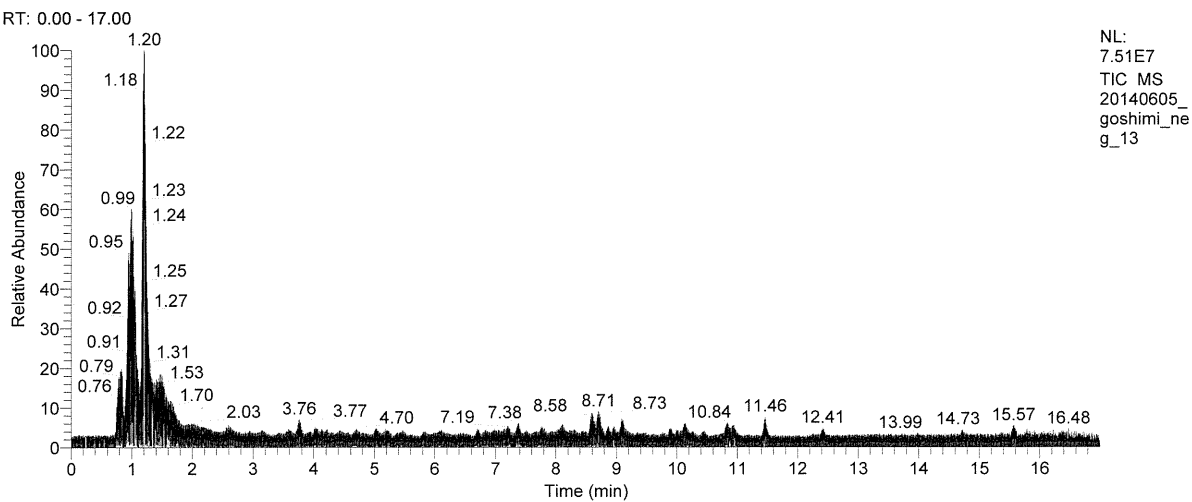
NIB-360



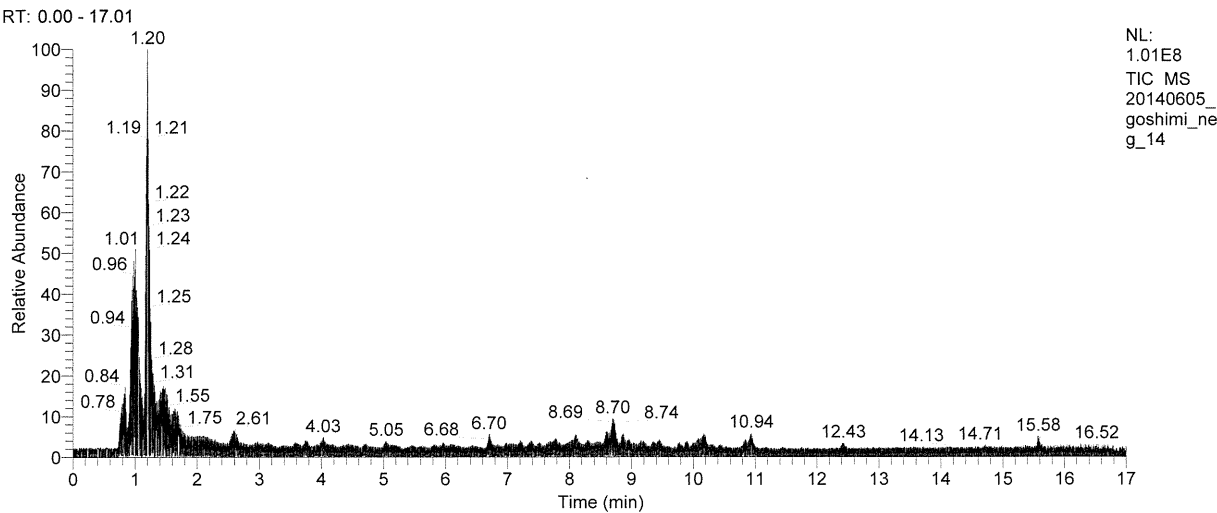
NIB-437



NIB-446

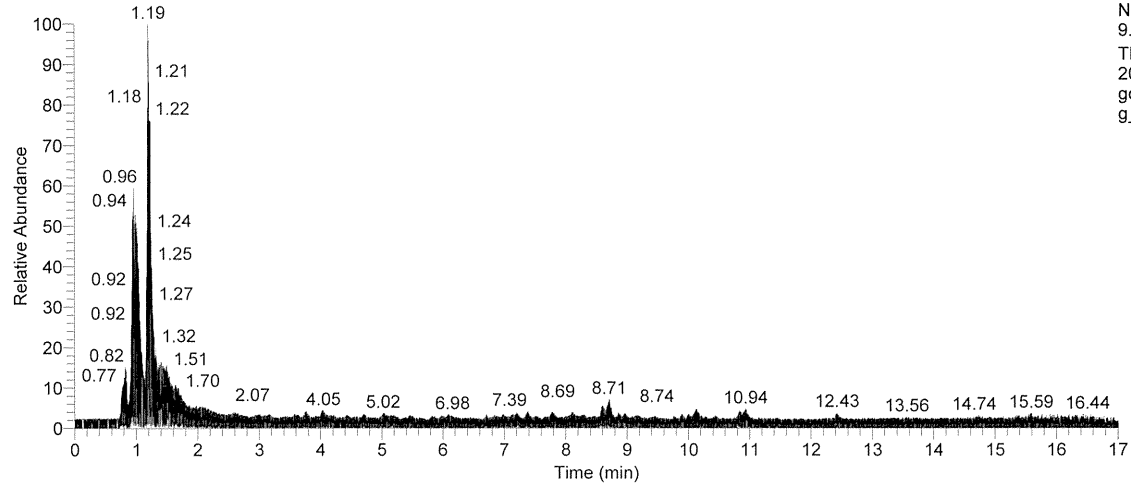


NIB-646



NIB-737

RT: 0.00 - 17.00



NL:
9.23E7
TIC MS
20140605_
goshimi_ne
g_15

ゴミシ MS スペクトルリスト

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
0.79	165.0508 (3.90E6)		142.0350(25), 124.0243(2.15E6; 100)				
	184.0454 (5.22E6)		161.0292(40), 143.0186(1.16E6; 100), 124.0241(85,), 101.0080(10)				
				0.8	343.0369 (2.21E6)		201.0253(5.82E5; 100),
					201.0253		157.0353(2.51E5; 100)
0.9	258.1099 (7.95E5)		168.0655(5), 104.1068(4.12E5; 100.), 96.0442(7)				
				0.93	191.0558 (5.30E6)	C7H11O6	173.0453(60, C7H9O5), 127.0401(70, C6H7O3), 111.0452(30, C6H7O2), 93.0347(50, C6H5O), 85.0296(4.34E5; 100,)
				0.99	191.0196 (2.92E7)	C6H7O7	173.0089(15, C6H5O6), 111.0088(1.60E7; 100, C5H3O3)
				1.2	191.0196 (4.57E7)	C6H7O7	173.0090(8, C6H5O6), 111.0088(5.96E7; 100, C5H3O3), 87.0089(2, C3H3O3)
1.2	210.0611 (2.80E6)	C6H12O7N	193.0343(60, C6H9O7), 175.0236(2.06E5; 100, C6H7O6), 165.0657(7,), 147.0287(12, C5H7O5), 136.0392(15)				
1.21	284.0979 (7.53E5)	C9H18O9N	267.0711(10, C9H15O9), 249.0605(2.17E5; 100, C9H13O8)				
				1.48	347.0616 (4.42E6)	C13H15O11	191.0193(2, C6H7O7), 173.0088(50, C6H5O6), 111.0086(2.44E6; 100, C5H3O3)
				1.56	391.0328 (4.92E5)		
				1.62	391.1245 (9.45E5)	C16H23O11	373.0218(5), 229.0715(35), 217.0158(3.55E5; 100), 211.0609(65), 193.0503(40), 185.0816(8), 167.0347(25), 149.0606(15), 141.0555(20), 123.0451(8),
				1.67	205.0353 (1.09E6)	C7H9O7	173.0088(45, C6H5O6), 143.0349(7, C6H7O4), 111.0086(2.44E6; 100, C5H3O3), 87.0088(5, C3H3O3)
				2.58	153.0191 (5.02E6)	C7H5O4	109.0295(4.06E4; 100, C6H5O2)
				3	313.0929 (6.28E5)	C15H13O4N4	269.1032(3.97E4; 100, C14H13O2N4), 161.0455(70, C7H5ON4), 113.0246(8, C5H5O3), 101.0246(12, C2H5ON4)
				3.04	475.1454 (4.27E5)	C21H23O9N4	431.1555(1.08E5; 100, C20H23O7N4), 269.1031(25, C14H13O2N4), 161.0454(5, C7H5ON4)
				3.1	353.0880 (6.13E5)	C17H13O5N4	191.0557(2.56E5; 100), 179.0347(45), 135.0451(5, C8H7O2)

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
				3.44	375.1296 (2.24E6)	C17H18O6N4	213.0764(9.87E5; 100, C10H13O5), 169.0867(12, C9H13O3)
				3.59	443.1918 (4.70E5)	C21H31O10	425.1818(35, C21H29O9), 281.1391(40, C15H21O5: -Glc), 263.1288(20, C15H19O4), 237.1494(7.25E3; 100, C14H21O3), 219.1389(55, C14H19O2), 189.1281(30, C13H17O), 179.0558(25, C6H11O6), 161.0453(60, C6H9O5), 143.0348(40, C6H7O4)
3.75	424.1818 (6.66E5)	C17H30O11N ([M+NH4]+)	406.1702(25, C17H28O10N), 389.1436(15, C17H25O10), 227.0911(1.17E5; 100, C11H15O5), 195.0650(10, C10H11O4)	3.71	441.1168 (2.11E6)	C17H26O11 Cl ([M+Cl]-)	405.1395(1.31E4; 100, C17H25O11), 243.0873(80, C11H15O6)
	429.1367	C17H26O11Na			405.1401	C17H25O11 ([M-H]-)	373.1136(25, C16H21O10), 345.1552(10, C16H25O8), 314.1438(8,), 285.0979(5, C13H17O7), 243.0872(5.48E4; 100, C11H15O6: -Glc), 225.0766(10, C11H13O5), 179.0557(30, C6H11O6), 155.0347(15, C7H7O4), 141.0555(12, C7H9O3), 123.0451(8, C7H7O2)
				3.76	289.0721 (1.24E6)	C16H9O2N4	245.0820(1.46E5; 100, C15H9N4), 231.0300(5, C13H3ON4), 205.0505(40, C12H5N4), 179.0348(15, C10H3N4), 165.0192(5, C9HN4), 125.0245(7,)
					353.0883 (5.49E5)	C17H13O5N4	191.0559(9.68E5; 100, C8H7O2N4), 179.0350(3, C10H3N4)
				3.79	389.1094 (8.48E5)	C17H17O7N4	345.1190(2.67E5; 100, C16H17O5N4), 209.0455(25, C11H5ON4), 183.0661(5, C10H7N4), 165.0556(15, C9H9O3), 121.0659(10, C8H9O)
				3.91	507.1719 (8.65E5)	C21H31O14	357.1189(5.52E4; 100, C16H21O9), 327.1085(45, C15H19O8: -Glc(+OH)), 301.1293(15, C14H21O7), 283.1187(55, C14H19O6), 213.0768(5, C10H13O5), 195.0662(10, C10H11O4), 179.0559(10, C6H11O6), 177.0555(15, C10H9O3)
4	306.0609 (5.20E5)	C14H12O7N	288.0499(1.79E5; 100, C14H10O6N), 262.0708(10, C13H12O5N), 168.0290(25, C7H6O4N), 152.0341(15, C7H6O3N)	3.98	304.0457 (5.31E6)	C14H10O7N	260.0565(6.44E4; 100, C13H10O5N), 216.0666(7, C12H10O3N), 166.0144(85, C7H4O4N), 153.0192(40, C7H5O4), 150.0196(80, C7H4O3N), 137.0244(10, C7H5O3), 122.0248(40, C6H4O2N), 109.0296(20,), 106.0299(15)
				4.13	381.1920 (7.38E5)	C21H25O3N4	363.1809(20, C21H23O2N4), 337.2018(2.40E5; 100, C20H25ON4),

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
							317.1757(15, C20H21N4)
				4.32	449.1657 (6.42E5)	C19H29O12 ([M+AcO]-)	389.1452(20, C17H25O10), 227.0924(3.46E5; 100, C11H15O5: 389-Glc)
					425.1214	C17H26O10 Cl ([M+Cl]-	406.1436(20), 365.1966(1.11E4; 100)
				4.38	220.0614 (1.33E6)		176.0714(1.42E5; 100)
				4.55	337.0929 (8.33E5)	C16H17O8	191.0558(7, C7H11O6), 173.0452(2.68E5; 100, C7H9O5), 163.0398(10, C9H7O3)
				4.68	403.1248 (8.36E5)	C17H23O11	371.0980(1.00E5; 100, C16H19O10), 333.0825(5, C13H17O10), 223.0610(50, C11H11O5), 179.0558(30, C6H11O6), 161.0453(5, C6H9O5), 143.0349(3, C6H7O4), 121.0295(5, C7H5O2)
5.03	290.0659 (6.74E5)	C14H12O6N	272.0554(3.18E5; 100, C14H10O5N), 246.0764(10, C13H12O4N)	5.02	288.0511 (5.51E6)	C14H10O6N	270.0410(20, C14H8O5N), 244.0617(1.33E5; 100, C13H10O4N), 200.0716(15, C12H10O2N), 150.0197(50, C7H4O3N), 137.0245(15, C7H5O3), 106.0299(10,), 93.0347(5)
	272.0555	C14H10O5N	254.0448(2.10E5; 100, C14H8O4N)				
				5.54	347.1707 (1.40E6)	C16H27O8	329.1605(45, C16H25O7), 303.1812(1.24E5; 100, C15H27O6), 211.1338(8, C12H19O3), 185.1181(15, C10H17O3: -Glc), 161.0454(80, C6H9O5), 159.0298(30, C6H7O5), 143.0350(10, C6H7O4), 129.0193(8, C5H5O4), 113.0245(45, C5H5O3), 101.0245(25, C4H5O3)
				5.78	437.1452 (8.37E5)	C21H25O10	325.0928(6.33E4; 100, C15H17O8), 307.0825(5, C15H15O7), 265.0719(80, C13H13O6), 235.0612(80, C12H11O5), 205.0506(3, C11H9O4), 163.0399(3, C9H7O3)
				5.96	187.0974 (7.06E5)	C9H15O4	125.0973(1.83E5; 100, C8H13O)
				6.72	549.2335 (5.04E5)	C28H37O11	531.2228(4.47E4; 100, C28H35O10), 513.2124(45, C28H33O9), 505.2437(10, C27H37O9), 495.2019(25, C28H31O8), 487.2331(8, C27H35O8), 477.1914(10, C28H29O7), 469.2228(15, C27H33O7), 451.2123(30, C27H31O6), 433.2015(8, C27H29O5), 407.2224(20, C26H31O4), 389.2118(8, C26H29O3), 279.1388(5, C19H19O2)

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
				6.98	543.2230 (5.44E5)	C29H35O10	525.2120(10, C29H33O9), 498.2207(12,), 480.2102(5), 445.1862(1.34E5; 100, C24H29O8), 427.1757(10, C24H27O7), 417.1913(8, C23H29O7), 405.1550(8, C21H25O8), 383.1861(5, C23H27O5), 355.1912(5, C22H27O4), 319.1184(5, C17H19O6), 287.0924(3, C16H15O5), 273.1133(6, C16H17O4), 243.1026(5, C15H15O3)
				7.09	365.1969 (5.33E5)	C20H29O6	347.1858(70, C20H27O5), 321.2067(1.02E5; 100, C19H29O4), 301.1806(35, C19H25O3)
				7.12	543.2232 (4.45E5)	C29H35O10	525.2124(15, C29H33O9), 499.2332(10, C28H35O8), 481.2228(10, C28H33O7), 445.1862(1.48E5; 100, C24H29O8), 427.1760(8, C24H27O7), 417.1913(6, C23H29O7), 405.1551(2, C21H25O8), 383.1863(3, C23H27O5), 355.1915(2, C22H27O4), 319.1184(3, C17H19O6), 287.0925(3, C16H15O5), 273.1133(4, C16H17O4), 243.1025(3, C15H15O3)
				7.24	639.1740 (4.60E5)	C29H35O14S	557.2019(3.80E5;100, C29H33O11), 513.2124(2, C28H33O9), 455.1706(10, C25H27O8), 417.1917(3, C23H29O7)
					557.2018	C29H33O11	539.1918(10, C29H31O10), 513.2124(15, C28H33O9), 499.1606(20, C26H27O10), 495.2018(15, C28H31O8), 481.1502(20, C26H25O9), 455.1707(3.04E4; 100, C25H27O8), 437.1603(15, C25H25O7), 393.1705(3, C24H25O5)
				7.41	605.2587 (2.90E5)	C31H41O12 ([M+AcO]−)	559.2175(5, C29H35O11), 545.2381(1.72E5; 100, C29H37O10), 527.2277(15, C29H35O9), 509.2173(5, C29H33O8), 447.2002(2, C24H31O8), 429.1912(30, C24H29O7), 411.1807(30, C24H27O6), 367.1910(10, C23H27O4)
					581.2153 (2.11E5)	C29H38O10 Cl ([M+Cl]−)	545.2380(3.25E4; 100, C29H37O10), 527.2279(35, C29H35O9), 509.2173(30, C29H33O8), 491.2068(10, C29H31O7), 465.2281(5, C28H33O6), 447.2167(5, C28H31O5), 429.1913(40, C24H29O7), 411.1808(60, C24H27O6), 367.1911(45, C23H27O4)

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
7.68	288.2897 (5.17E5)	C17H38O2N	270.2789(25, C17H36ON), 177.0674(7,), 106.0860(5.17E4; 100, C4H12O2N), 88.0754(15, C4H10ON)				
				7.69	607.2756 (3.28E5)	C31H43O12 ([M+AcO]-)	547.2541(1.83E5; 100, C29H39O10), 529.2436(60, C29H37O9), 525.2126(10, C29H33O9), 511.2332(30, C29H35O8), 467.2437(3, C28H35O6)
					583.2314 (3.28E5)	C29H40O10 Cl ([M+Cl]-	547.2538(1.63E4; 100, C29H39O10), 529.2434(90, C29H37O9), 511.2329(80, C29H35O8), 485.2533(10, C28H37O7), 467.2435(25, C28H35O6)
7.87	288.2897 (7.32E5)	C17H38O2N	270.2789(1.16E5; 100, C17H36ON), 244.2632(10, C15H34ON), 177.0673(2), 106.0860(20, C4H12O2N), 102.0910(8, C5H12ON), 88.0754(5, C4H10ON)				
				7.8	242.1761 (1.22E6)	C13H24O3N	225.1493(1.43E5; 100, C13H21O3), 181.1593(50, C12H21O)
				8.02	329.2334 (1.46E6)	C18H33O5	311.2228(70, C18H31O4), 293.2122(25, C18H29O3), 229.1445(2.75E4; 100, C12H21O4), 211.1338(75, C12H19O3), 171.1025(25, C9H15O3)
				8.08	531.2236 (4.15E5)	C28H35O10	513.2117(80, C28H33O9), 495.2015(85, C28H31O8), 477.1909(30, C28H29O7), 469.2226(20, C27H33O7), 451.2117(4.43E4; 100, C27H31O6), 433.2015(40, C27H29O5), 415.1909(15, C27H27O4), 407.2221(50, C26H31O4), 389.2117(35, C26H29O3), 341.1389(13, C20H21O5), 295.1338(10, C19H19O3), 257.1180(15, C16H17O3)
				8.53	623.1802 (9.56E5)		605.1696(2), 559.2181(7), 541.2073(1.02E6; 100), 497.2181(3), 439.1761(25)
					541.2079	C29H33O10	523.1968(55, C29H31O9), 497.2174(40, C28H33O8), 483.1655(50, C26H27O9), 479.2068(20, C28H31O7), 465.1548(35, C26H25O8), 439.1756(1.65E4; 100, C25H27O7), 421.1651(50, C25H25O6), 395.1857(12, C24H27O5), 377.1753(15, C24H25O4), 365.1390(15, C22H21O5),
				8.61	633.2911 (3.64E5)	C33H45O12	573.2693(10, C31H41O10), 531.2588(3.18E5; 100, C29H39O9), 513.2485(5, C29H37O8), 495.2379(3, C29H35O7)
					531.2596	C29H39O9	513.2484(8.66E4; 100, C29H37O8), 495.2384(15, C29H35O7), 469.2592(8, C28H37O6), 337.1653(25, C18H25O6), 211.0973(5,

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
							C11H15O4)
				8.66	647.2705 (1.04E6)	C33H43O13 ([M+AcO]−	587.2495(2.41E5; 100, C31H39O11), 569.2389(35, C31H37O10), 527.2285(90, C29H35O9), 509.2180(85, C29H33O8), 491.2075(30, C29H31O7), 465.2283(15, C28H33O5), 447.2176(20, C28H31O5)
					623.2256	C31H40O11 Cl ([M+Cl]−	
8.73	608.3065 (6.53E5)	C31H46O11N ([M+NH4]+)	573.2682(65, C31H41O10), 531.2579(5, C29H39O9), 513.2472(6.53E5; 100, C29H37O8), 471.2369(5, C27H35O7)	8.72	649.2865 (2.19E6)	C33H45O13 ([M+AcO]−	589.2651(8.79E5; 100, C31H41O11), 571.2549(35, C31H39O10), 553.2446(55, C31H37O9), 529.2370 (5,), 509.2546(20, C30H37O7)
	573.2691	C31H41O10	513.2472(1.72E5; 100, C29H37O8), 495.2370(3, C29H35O7), 453.2266(5, C27H33O6)		625.2416	C31H42O11 Cl ([M+Cl]−	589.2643(65, C31H41O11), 571.2539(55, C31H39O10), 553.2435(70, C31H37O9), 542.2104(10,), 528.2316(25), 509.2529(9.24E4; 100, C30H37O7), 492.2109(10), 467.2437(7), 447.2173(15, C28H31O5)
				8.86	541.2070 (6.55E5)	C29H33O10	523.1973(15, C29H31O9), 497.2182(75, C28H33O8), 483.1653(40, C26H27O9), 479.2068(10, C28H31O7), 465.1556(20, C26H25O8), 439.1763(3.00E4; 100, C25H27O7), 421.1659(25, C25H25O6), 395.1869(8, C24H27O5), 365.1396(15, C22H21O5),
				8.87	633.2539 (3.12E5)	C32H41O13	573.2330(5.67E4; 100, C30H37O11), 531.2230(5, C28H35O10), 513.2123(30, C28H33O9)
				8.96	541.2070 (3.97E5)	C29H33O10	523.1964(12, C29H31O9), 497.2172(3.05E5; 100, C28H33O8), 479.2068(10, C28H31O7), 439.1763(7, C25H27O7)
				9.05	607.2761 (3.64E5)	C31H43O12 ([M+AcO]−	547.2541(3.31E5; 100, C29H39O10), 529.2437(25, C29H37O9), 511.2332(10, C29H35O8)
					583.2318 (3.72E5)	C29H40O10 Cl ([M+Cl]−	547.2539(1.10E4; 100, C29H39O10), 529.2437(98, C29H37O9), 511.2332(75, C29H35O8), 485.2540(15, C28H37O7), 467.2432(35, C28H35O6), 427.2110(5, C25H31O5), 401.1961(10, C23H29O5), 354.1469(5, C21H22O5)
9.92	415.2112 (2.81E7)	C24H31O6	400.1882(25, C23H28O6), 384.1931(2.14E5; 100, C23H28O5), 374.1683(15,), 359.1492(20)				

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
	433.2219	C24H33O7 ([M+H] ⁺) Schisandrin	415.2115(1.39E6; 100, C24H31O6)				
	450.2487	C24H36O7N ([M+NH4] ⁺)	433.2221(1.35E3; 100), 415.1900(30), 400.				
	384.1929	C23H28O5	369.1700(1.40E6; 100, C22H25O5), 353.1752(60, C22H25O4), 338.1521(12, C21H22O4),				
	369.1694	C22H25O5	354.1460(25, C21H22O5), 338.1512(1.05E6; 100, C21H22O4), 310.1563(10, C20H22O3)				
				10.01	715.2963 (3.60E5)	C37H47O14 ([M+AcO] ⁻)	655.2741(7.67E4; 100, C35H43O12), 613.2640(20, C33H41O11), 595.2535(12, C33H39O10), 573.2330(10, C30H37O11), 555.2224(40, C30H35O10), 531.2226(7, C28H35O10), 513.2118(90, C28H33O9), 495.2015(15, C28H31O8), 477.1909(5, C28H29O7)
					691.2521	C35H44O12 Cl ([M+Cl] ⁻)	
				10.09	647.2705 (5.97E5)	C33H43O13 ([M+AcO] ⁻)	587.2491(75, C31H39O11), 569.2387(3, C31H37O10), 527.2282(1.64E5; 100, C29H35O9), 509.2180(15, C29H33O8), 491.2073(5, C29H31O7)
					623.2256 (8.83E5)	C31H40O11 Cl ([M+Cl] ⁻)	587.2485(15, C31H39O11), 563.2059(20), 527.2275(2.96E4; 100, C29H35O9), 509.2170(35, C29H33O8), 491.2064(20, C29H31O7), 483.2371(3, C28H35O7), 465.2280(5, C28H33O5), 447.2169(20, C28H31O5)
10.15	548.2492 (6.48E5)	C28H38O10N ([M+NH4] ⁺)	485.2166(70, C27H33O8), 401.1590(4.19E5; 100, C22H25O7), 383.1487(5, C22H23O6)				
	401.1596	C22H25O7 Gomisin N	383.1488(3.51E5; 100, C22H23O6), 371.1490(7, C21H23O6), 357.1333(15, C20H21O6), 341.1020(25, C19H17O6)				
10.2	608.3063 (2.48E5)	C31H46O11N ([M+NH4] ⁺)	573.2679(2.53E5; 100, C31H41O10), 555.2576(25, C31H39O9), 537.2471(5, C31H37O8), 513.2470(2.53E5E5; 100, C29H37O8), 495.2368(12, C29H35O7), 471.2367(5, C27H35O7), 453.2261(15, C27H33O6)	10.19	649.2861 (9.97E5)	C33H45O13 ([M+AcO] ⁻)	589.2642(3.54E5; 100, C31H41O11), 571.2540(13, C31H39O10), 553.2433(15, C31H37O9), 509.2537(3, C30H37O7)
					625.2411 (1.22E6)	C31H42O11 Cl ([M+Cl] ⁻)	589.2646(9.58E4; 100, C31H41O11), 571.2542(65, C31H39O10),

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
							553.2437(70, C31H37O9), 542.2104(10,), 528.2322(25), 509.2537(90, C30H37O7), 469.2225(7, C27H33O7), 449.2328(5, C28H33O5)
10.28	389.1953 (5.16E5)	C22H29O6	357.1695(1.46E5; 100, C21H25O5), 325.1433(60, C20H21O4), 319.1176(45, C17H19O6), 301.1070(12, C17H17O5), 287.0913(30, C16H15O5), 221.1172(10, C13H17O3)				
				10.41	487.3424 (3.15E5)	C30H47O5	469.3323(2.80E4; 100, C30H45O4)
					607.1851 (3.81E5)		547.2543(25), 543.2230(65), 525.2123(7.60E4; 100), 507.2020(5), 481.2224(8), 463.2123(15)
				10.44	499.1971 (4.87E5)	C27H31O9	417.1549(10, C22H25O8), 399.1443(3.95E4; 100, C22H23O7), 385.1288(7, C21H21O7), 367.1183(13, C21H19O6), 325.1077(20, C19H17O5), 315.0871(10, C17H15O6)
10.49	434.2174 (2.06E6)	C23H32O7N ([M+NH4]+) Gomisin A	416.2140(2.43E4; 100), 415.2105(90), 399.1795(40, C23H27O6),				
	399.1805	C23H27O6	369.1682(1.84E5; 100, C22H25O5), 368.1613(65, C22H24O5), 357.1330(30, C20H21O6), 343.1172(20, C19H19O6), 337.1432(20, C21H21O4), 330.1094(8, C18H18O6)				
				10.61	299.1324 (8.63E5)	C11H23O9	281.1217(8.70E3; 100, C11H21O8), 217.1597(60), 205.1599(20)
10.83	415.2113 (5.95E5)	C24H31O6	400.1879(25, C23H28O6), 384.1928(1.43E5; 100, C23H28O5), 373.1645(20, C21H25O6), 359.1489(20, C20H23O6)				
				10.83	389.1967 (1.22E6)	C22H29O6	374.1731(2.91E5; 100, C21H26O6)
10.84	515.2272 (1.56E5)	C28H35O9	469.2216(20, C27H33O7), 385.1639(2.91E5; 100, C22H25O6), 355.1537(30, C21H23O5), 323.1276(5, C20H19O4)				
				10.84	531.2230 (5.38E5)	C28H35O10	401.1599(1.55E5; 100, C22H25O7)
10.85	391.2113 (2.43E5)	C22H31O6	359.1854(15, C21H27O5), 327.1593(12, C20H23O4), 237.1484(1.70E5; 100, C14H21O3), 205.1223(45, C13H17O2), 167.0702(10, C9H11O3)				
10.92	401.1961 (7.85E5)	C23H29O6 Gomisin N	386.1726(10, C22H26O6), 369.1699(1.41E5; 100, C22H25O5), 359.1495(20, C20H23O6), 345.1337(15, C19H21O6), 341.1751(15, C21H25O4), 337.1440(70, C21H21O4), 309.1490(12,				

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
			C20H21O3)				
	483.2381 (7.44E5)	C28H35O7	451.2112(2.54E5; 100, C27H31O6), 427.1747(50, C24H27O7), 414.1666(15, C23H26O7), 409.2006(15, C25H29O5), 394.1408(20, C23H22O6), 349.1069(8, C21H17O5), 262.1198(5, C15H18O4)				
	515.2278 (1.20E6)	C28H35O9	469.2213(20, C27H33O7), 385.1637(1.32E6; 100, C22H25O6), 355.1534(25, C21H23O5), 323.1273(5, C20H19O4)				
	555.2201 (4.05E5)	C28H36O10Na ([M+Na]⁺)	537.2082(8.93E4; 100, C28H34O9Na), 509.2134(90, C27H34O8Na), 491.2029(25, C27H32O7Na), 407.1456(10, C22H24O6Na)	10.94	531.2230 (5.38E5)	C28H35O10	401.1598(1.79E5; 100, C22H25O7)
					401.1603	C22H25O7	285.0766(2.91E5; 100, C16H13O5), 270.0532(15, C15H10O5), 257.0817(5, C15H13O4)
11.1	399.1801 (1.47E6)	C23H27O6	384.1563(10, C22H24O6), 369.1689(1.05E5; 100, C22H25O5), 368.1613(70, C22H24O5), 357.1332(30, C20H21O6), 343.1174(25, C19H19O6), 337.1432(15, C21H21O4), 330.1097(8, C18H18O6)				
11.24	401.1961 (4.94E6)	C23H29O6 Gomisin N	386.1725(10, C22H26O6), 369.1693(4.35E5; 100, C22H25O5), 359.1492(20, C20H23O6), 345.1334(15, C19H21O6), 341.1748(15, C21H25O4), 337.1437(65, C21H21O4), 309.1487(10, C20H21O3)				
	483.2383 (2.06E6)	C28H35O7	451.2112(2.49E5; 100, C27H31O6), 427.1747(50, C24H27O7), 414.1666(15, C23H26O7), 409.2007(15, C25H29O5), 394.1408(20, C23H22O6), 349.1069(8, C21H17O5), 262.1198(5, C15H18O4)				
	501.2487 (8.96E5)	C28H37O8	485.2161(95, C27H33O8), 483.2368(80, C28H35O7), 468.2134(8.48E3; 100, C27H32O7), 425.1952(90, C25H29O6), 418.1974(50, C23H30O7), 401.1947(55, C23H29O6), 343.1532(10, C20H23O5), 327.1589(20, C20H23O4)				
	523.2307 (7.66E5)	C28H36O8Na ([M+Na]⁺)	508.2051(8.34E4; 100, C27H33O8Na), 477.1869(20, C26H30O7Na), 441.1870(40, C23H30O7Na), 409.1608(35, C22H26O6Na), 386.1711(70, C20H27O6Na), 315.1216(5, C16H20O5Na)				

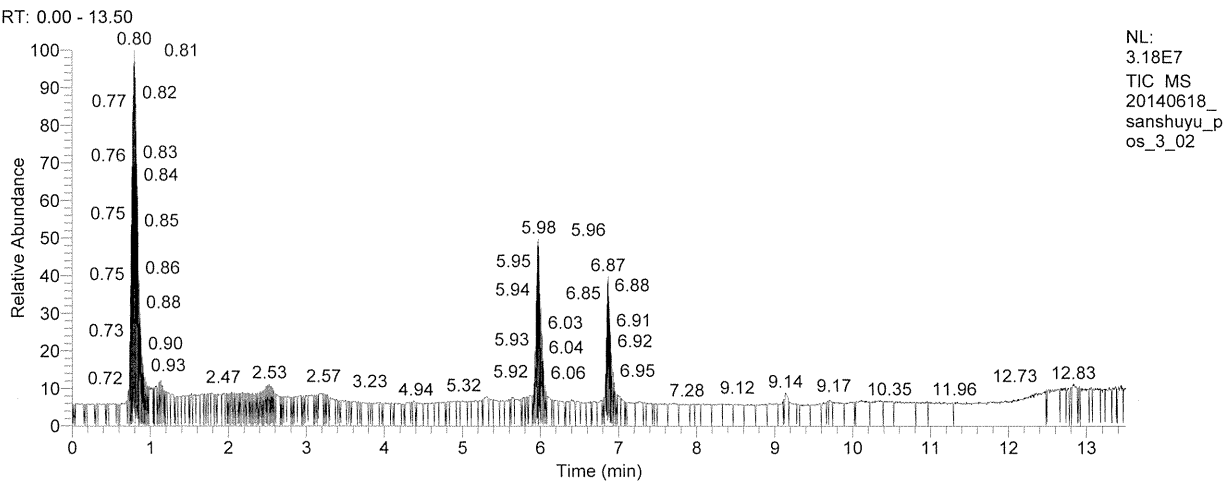
正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
11.37	399.1797 (8.41E5)	C23H27O6	384.1565(10, C22H24O6), 369.1690(3.88E5; 100, C22H25O5), 368.1617(65, C22H24O5), 357.1332(30, C20H21O6), 343.1175(25, C19H19O6), 337.1434(15, C21H21O4), 330.1097(8, C18H18O6)				
11.53	548.2854 (7.64E5)	C29H42O9N ([M+NH4]+)	431.2060(4.62E5; 100, C24H31O7)				
	431.2062	C24H31O7	413.1954(15, C24H29O6), 399.1797(30, C23H27O6), 387.1798(2.37E5; 100, C22H27O6), 372.1563(15, C21H24O6), 357.1693(15, C21H25O5)				
11.6	554.2389 (6.14E5)	C30H36O9N ([M+NH4]+)	453.1876(25, C26H29O7), 431.2056(30, C24H31O7), 415.1742(3.02E5; 100, C23H27O7), 387.1795(5, C22H27O6)				
	415.1753	C23H27O7	397.1646(15, C23H25O6), 383.1489(30, C22H23O6), 371.1489(8.60E5; 100, C21H23O6), 356.1256(10, C20H20O6), 341.1383(12, C20H21O5)				
11.69	532.2537 (2.32E5)	C28H38O9N ([M+NH4]+)	415.1744(2.40E5; 100, C23H27O7)				
	415.1748	C23H27O7	397.1644(15, C23H25O6), 383.1487(30, C22H23O6), 371.1488(2.73E5; 100, C21H23O6), 356.1254(10, C20H20O6), 341.1382(12, C20H21O5), 329.1020(8, C18H17O6)				
11.92	532.2537 (4.82E5)	C28H38O9N ([M+NH4]+)	415.1741(7.38E5; 100, C23H27O7)				
	415.1748	C23H27O7	397.1641(15, C23H25O6), 385.1641(20, C22H25O6), 373.1276(30, C20H21O7), 371.1484(4.88E5; 100, C21H23O6), 367.1537(5, C22H23O5), 343.1173(5, C19H19O6)				
	403.2113 (9.98E5)	C23H31O6	388.1874(15, C22H28O6), 371.1847(5.09E5; 100, C22H27O5), 340.1663(30, C21H24O4), 333.1329(40, C18H21O6), 301.1068(20, C17H17O5)				
11.99	554.2389 (6.67E5)	C30H36O9N ([M+NH4]+)	415.1737(2.41E5; 100, C23H27O7), 371.1477(2, C21H23O6)				
	415.1748	C23H27O7	397.1640(12, C23H25O6), 385.1639(20, C22H25O6), 373.1274(25, C21H25O6), 371.1483(9.84E5; 100, C21H23O6), 367.1535(3, C22H23O5), 343.1172(5, C19H19O6)				
12.08	532.2536 (1.35E6)	C28H38O9N ([M+NH4]+)	415.1749(5.87E5; 100, C23H27O7)				
	415.1748	C23H27O7	397.1640(25, C23H25O6), 385.1640(30, C22H25O6), 373.1276(25, C20H21O7), 371.1484(5.83E5; 100, C21H23O6), 367.1535(5,				

正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
			C22H23O5), 343.1172(10, C19H19O6)				
12.33	403.2113 (8.25E5)	C23H31O6	388.1875(15, C22H28O6), 371.1848(1.25E5; 100, C22H27O5), 340.1665(40, C21H24O4), 333.1331(30, C18H21O6), 301.1068(15, C17H17O5)				
				12.34	485.3270 (1.07E5)	C30H45O5	467.3157(2.62E4; 100, C30H43O4), 441.3367(50, C29H45O3), 423.3264(7, C29H43O2), 383.2950(15, C26H39O2), 345.2437(3, C22H33O3)
				12.36	471.3477 (4.37E5)	C30H47O4	453.3369(4.84E4; 100, C30H45O3), 441.3373(7, C29H45O3), 427.3580(7, C29H47O2), 411.3266(3, C28H43O2)
12.63	515.2275 (6.24E5)	C28H35O9 Gomisin B	469.2212(20, C27H33O7), 385.1636(1.98E5; 100, C22H25O6), 355.1534(25, C21H23O5), 323.1273(5, C20H19O4)				
13.45	417.2265 (8.28E6)	C24H33O6	402.2034(70, C23H30O6), 386.2085(15, C23H30O5), 370.1772(13, C22H26O5), 347.1487(1.19E5; 100, C19H23O6), 332.1254(5, C18H20O6), 316.1303(70, C18H20O5)				
13.87	401.1954 (4.81E6)	C23H29O6	386.1723(50, C22H26O6), 371.1848(50, C22H27O5), 370.1774(30, C22H26O5), 354.1462(10, C21H22O5), 340.1667(8, C21H24O4), 331.1176(1.04E5; 100, C18H19O6), 301.1066(30, C17H17O5), 300.0993(45, C17H16O5), 273.1122(5, C16H17O4)				
14	401.1953 (1.18E7)	C23H29O6	386.1721(50, C22H26O6), 371.1847(55, C22H27O5), 370.1772(30, C22H26O5), 354.1463(10, C21H22O5), 340.1665(5, C21H24O4), 331.1176(7.92E5; 100, C18H19O6), 301.1065(20, C17H17O5), 300.0991(30, C17H16O5), 273.1120(5, C16H17O4)				
				14.73	277.2174 (1.35E6)	C18H29O2	259.2069(25, C18H27O), 233.2274(1.57E4; 100, C17H29), 179.1803(8, C13H23)

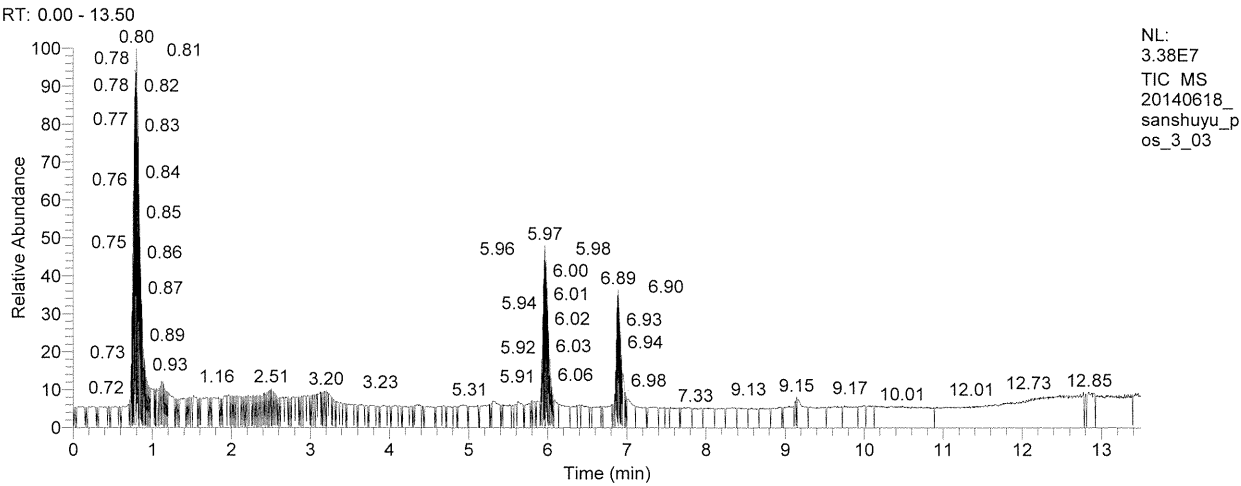
サンシュユ LC/MS データ (positive mode)

TIC

NIB-412



NIB-421



NIB-450

