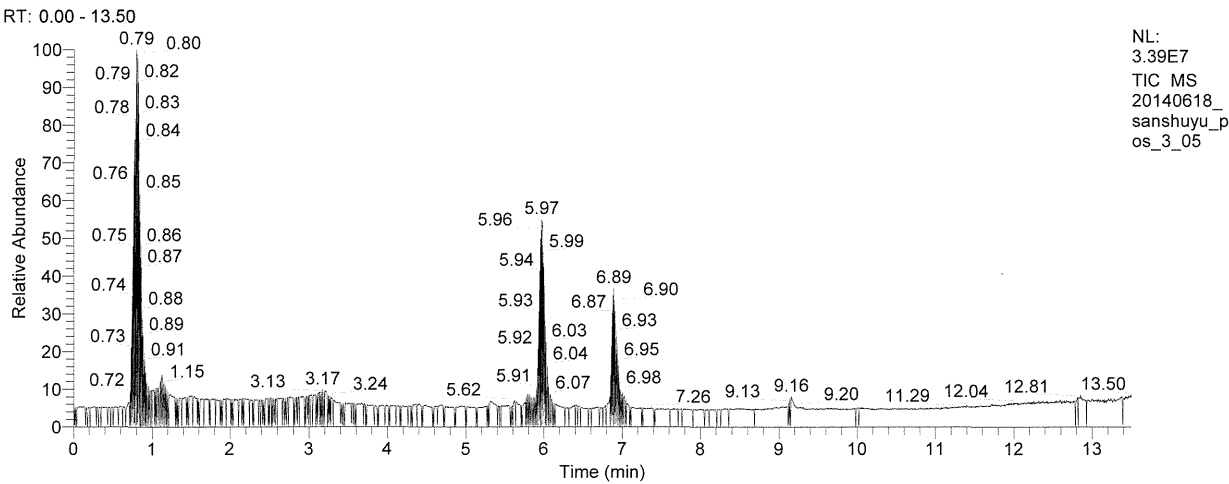
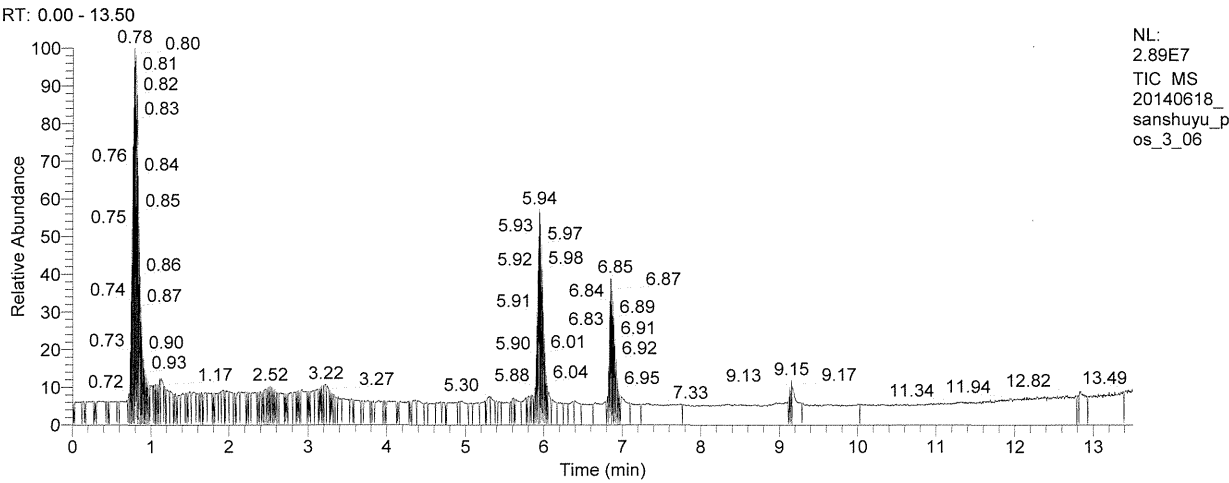


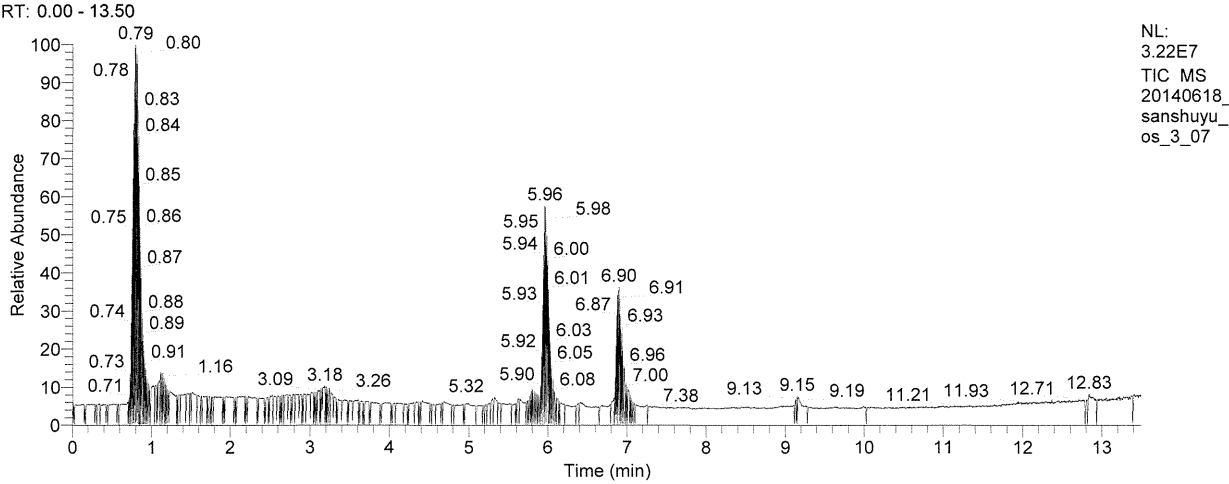
NIB-462



NIB-476

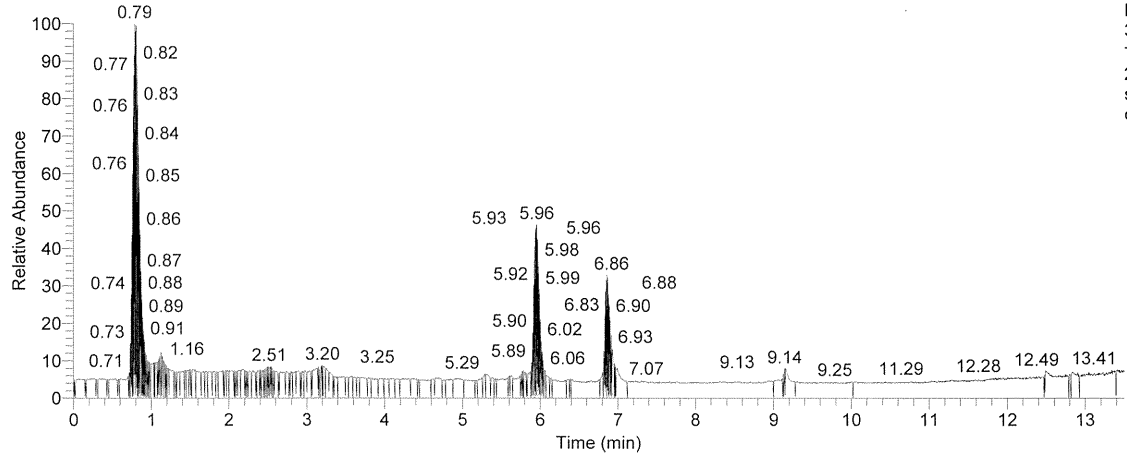


NIB-477



NIB-478

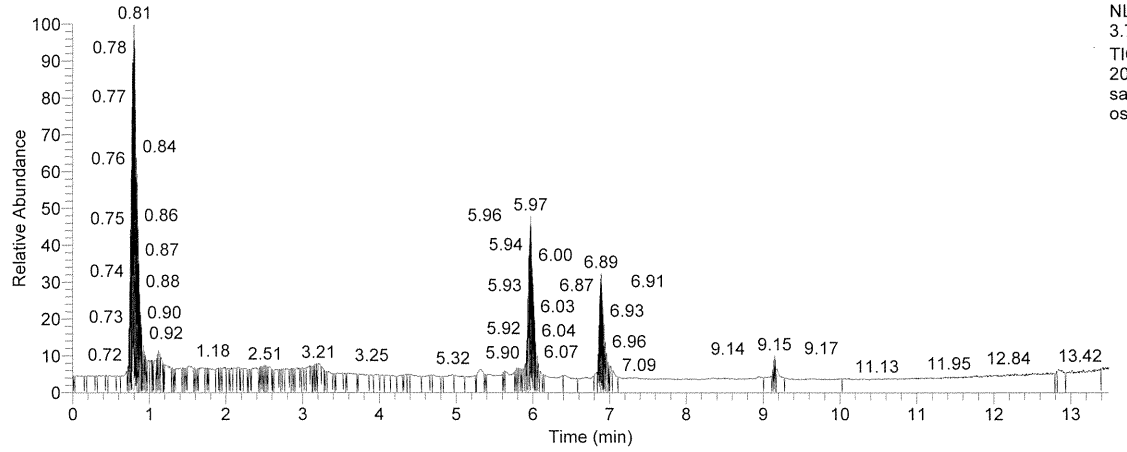
RT: 0.00 - 13.50



NL:
3.42E7
TIC MS
20140618_
sanshuyu_p
os_3_08

NIB-479

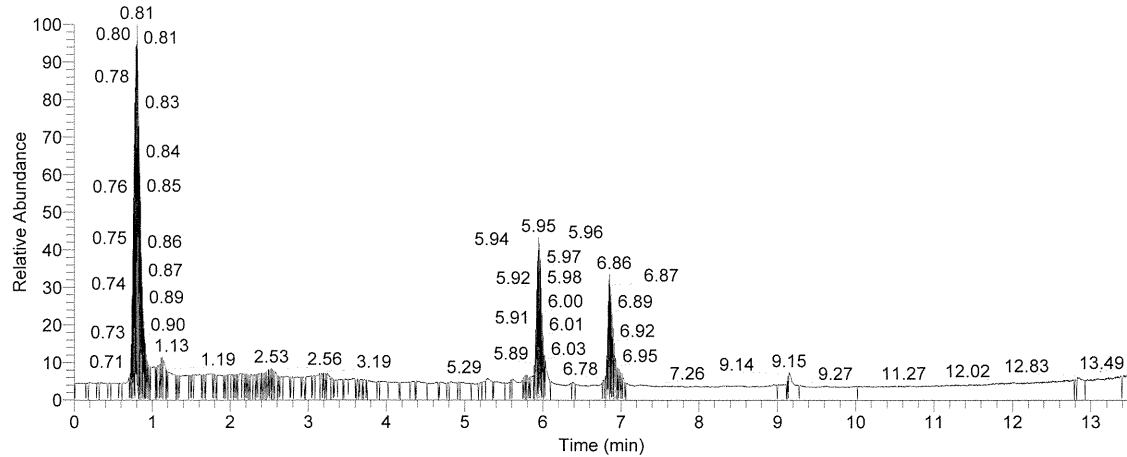
RT: 0.00 - 13.50



NL:
3.73E7
TIC MS
20140618_
sanshuyu_p
os_3_09

NIB-480

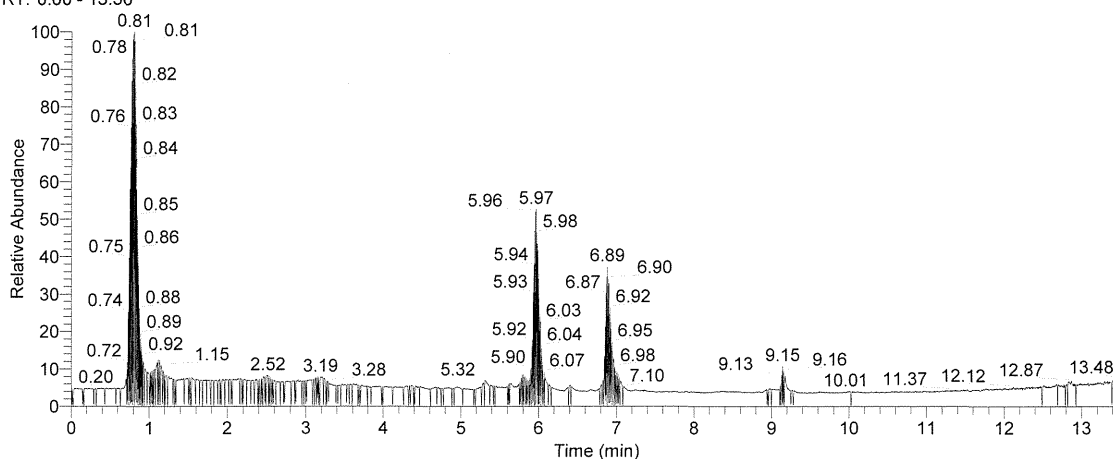
RT: 0.00 - 13.50



NL:
3.78E7
TIC MS
20140618_
sanshuyu_p
os_3_10

NIB-481

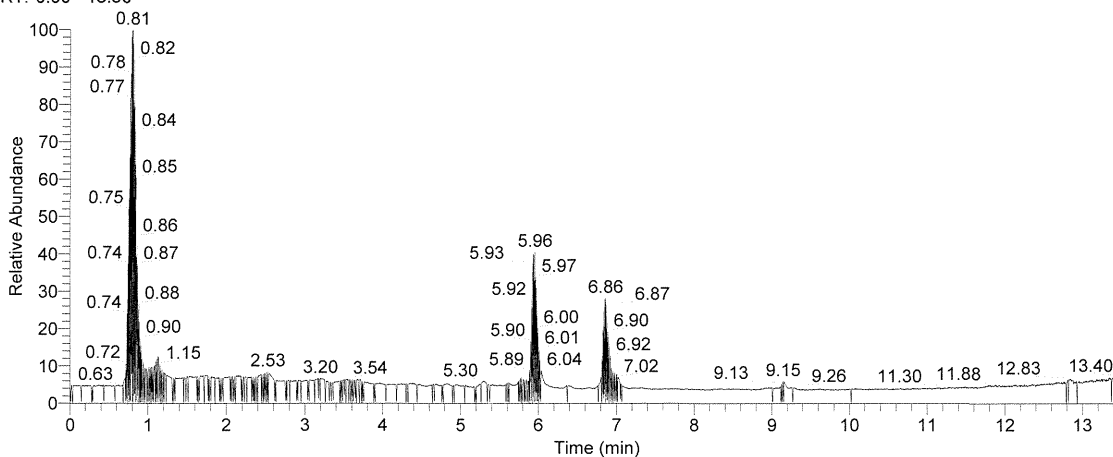
RT: 0.00 - 13.50



NL:
3.52E7
TIC MS
20140618_
sanshuyu_p
os_3_11

NIB-482

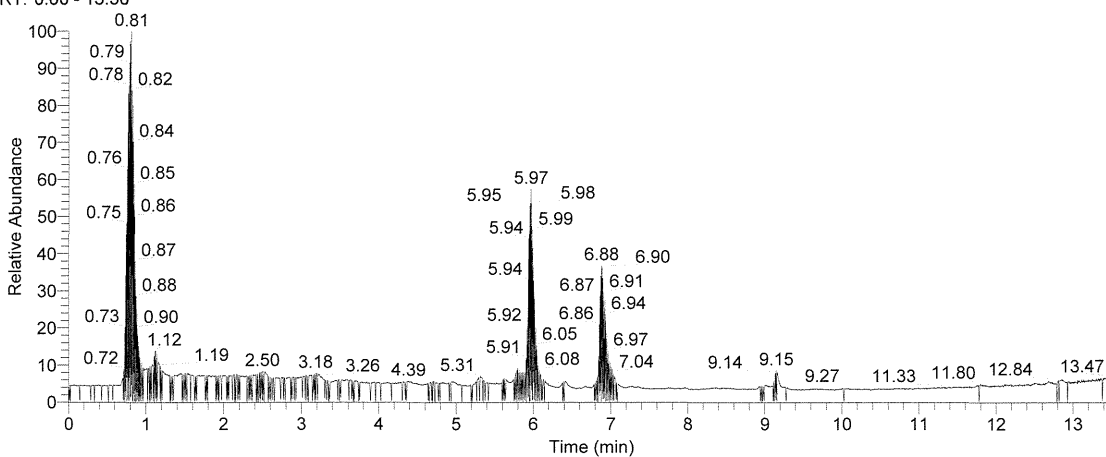
RT: 0.00 - 13.50



NL:
3.55E7
TIC MS
20140618_
sanshuyu_p
os_3_12

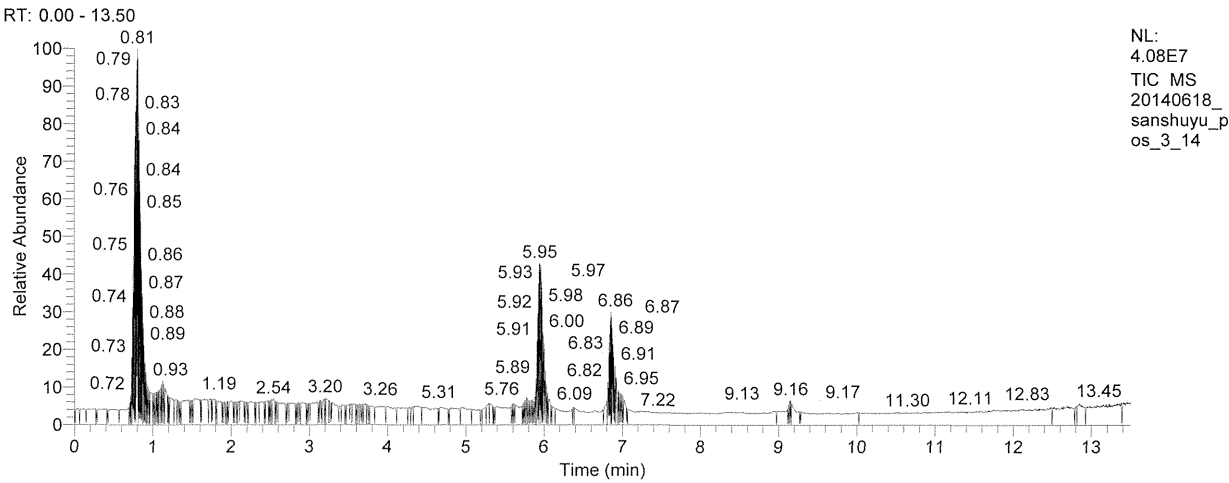
NIB-483

RT: 0.00 - 13.50

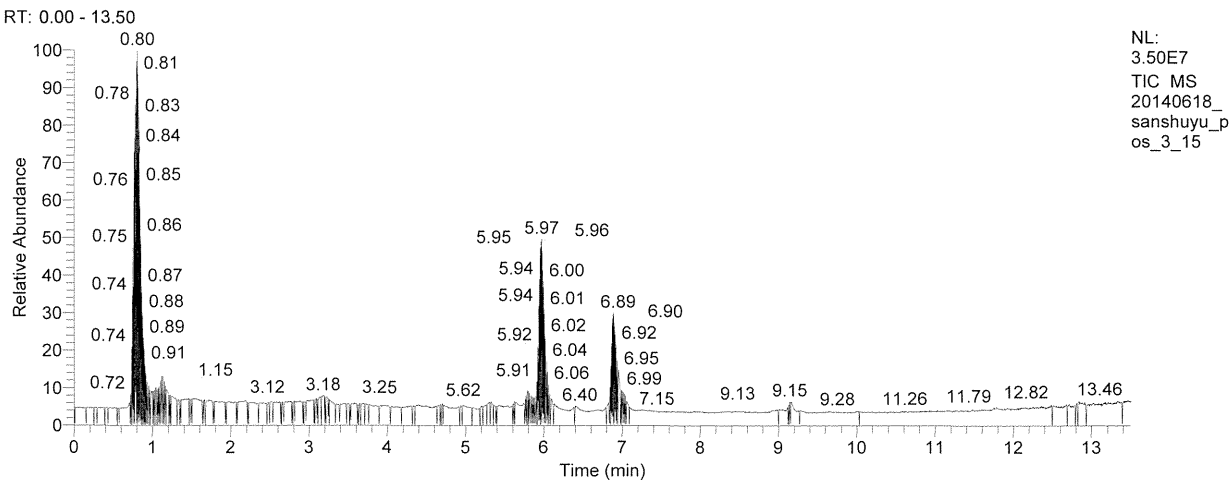


NL:
3.68E7
TIC MS
20140618_
sanshuyu_p
os_3_13

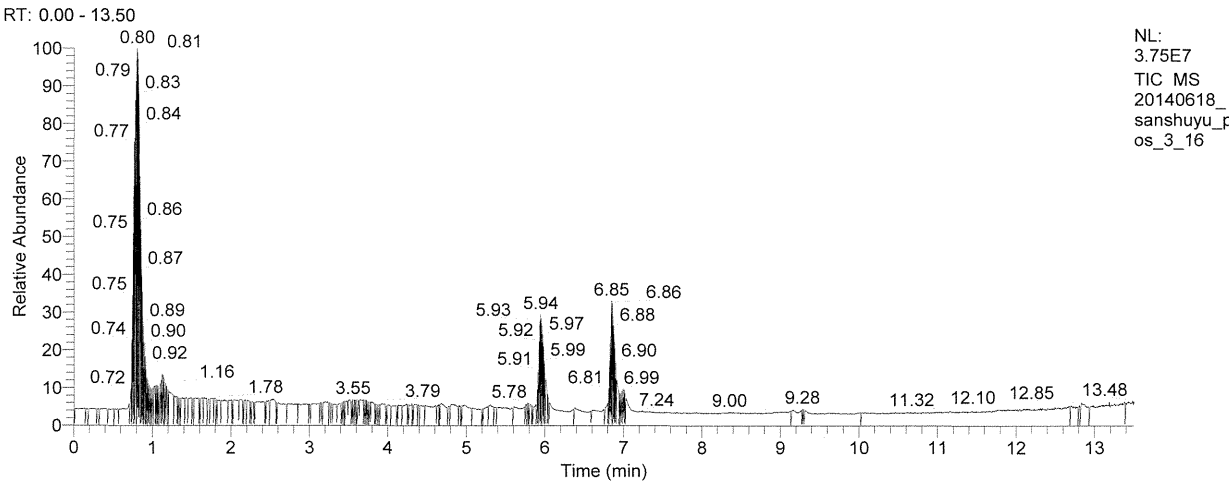
NIB-484



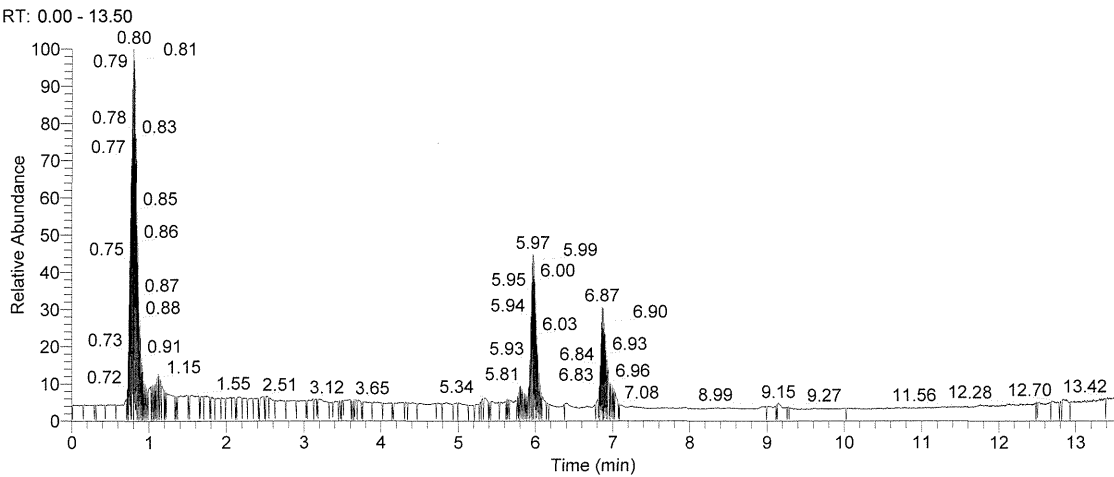
NIB-485



NIB-486

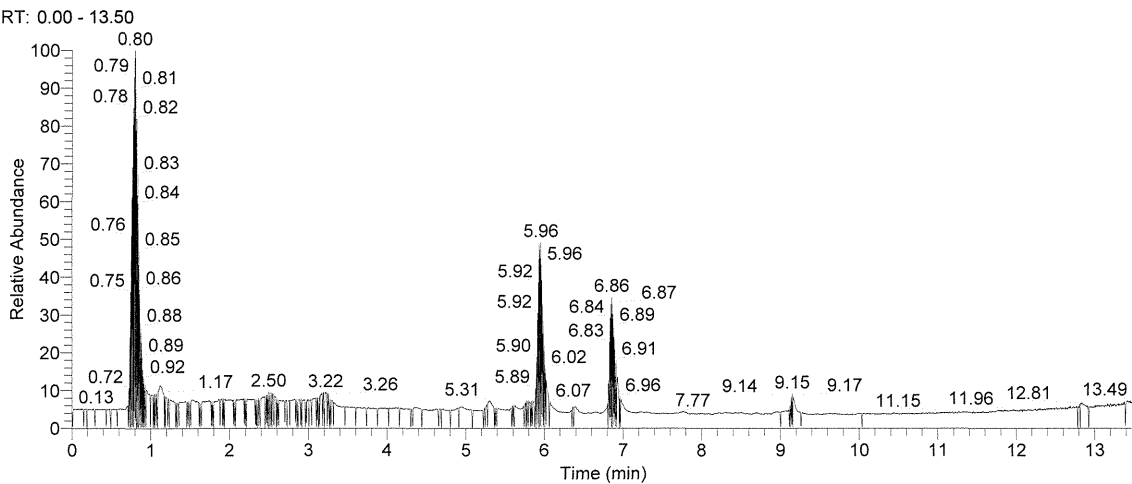


NIB-487



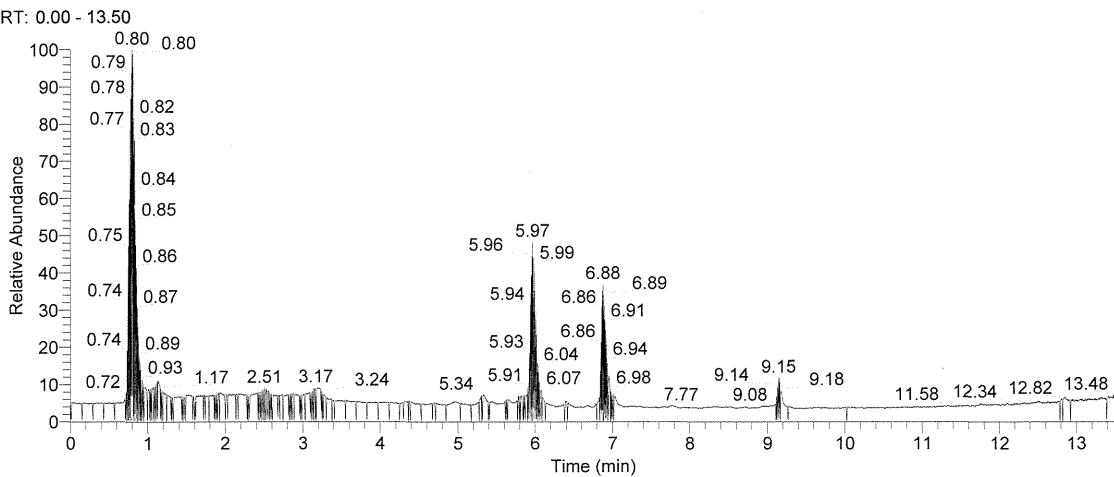
NL:
3.74E7
TIC MS
20140618_
sanshuyu_p
os_3_17

NIB-648



NL:
3.22E7
TIC MS
20140618_
sanshuyu_p
os_3_18

NIB-741

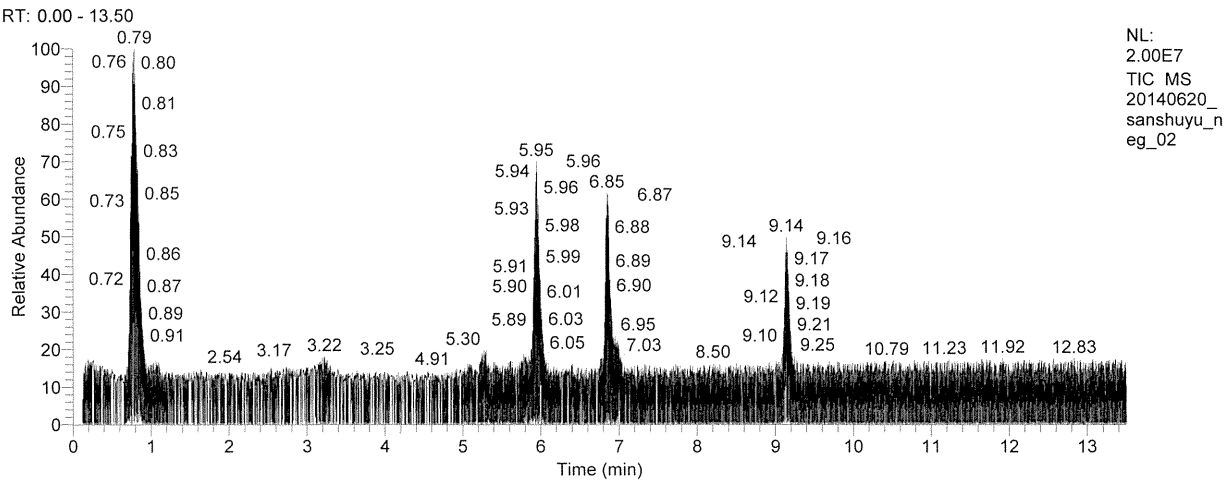


NL:
3.22E7
TIC MS
20140618_
sanshuyu_p
os_3_19

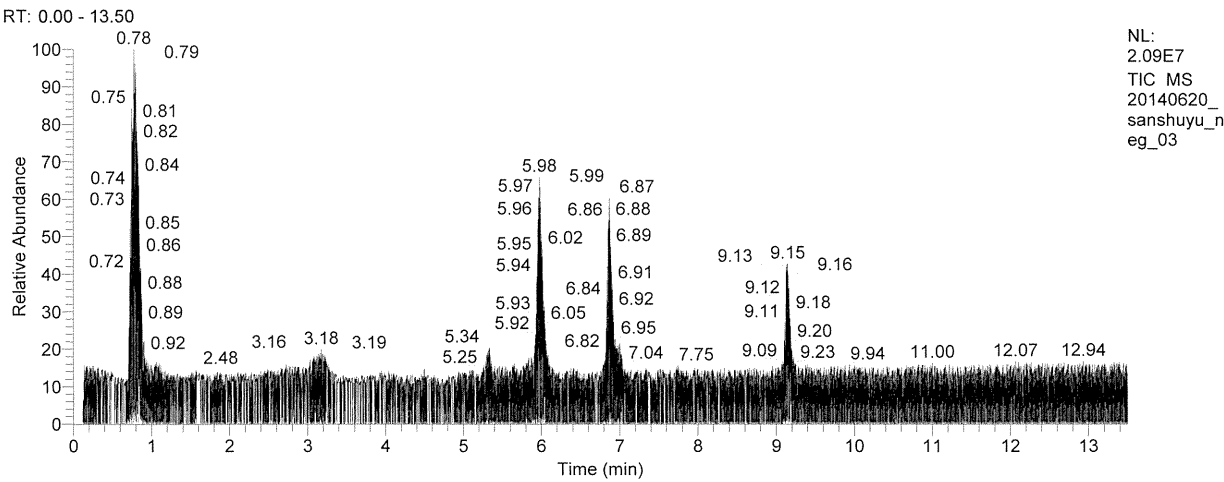
サンシュユ LC/MS データ(negative mode)

TIC

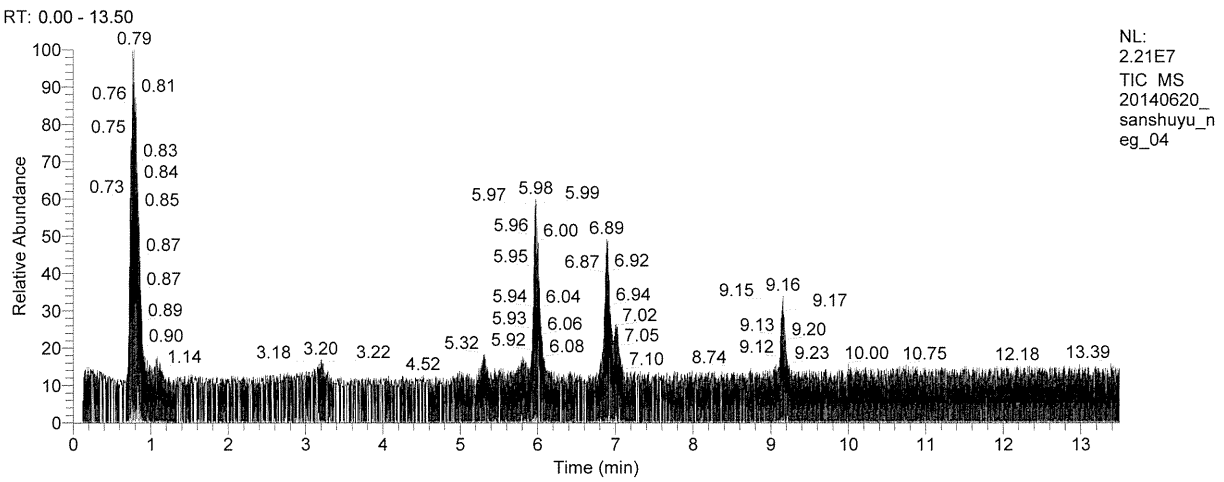
NIB-412



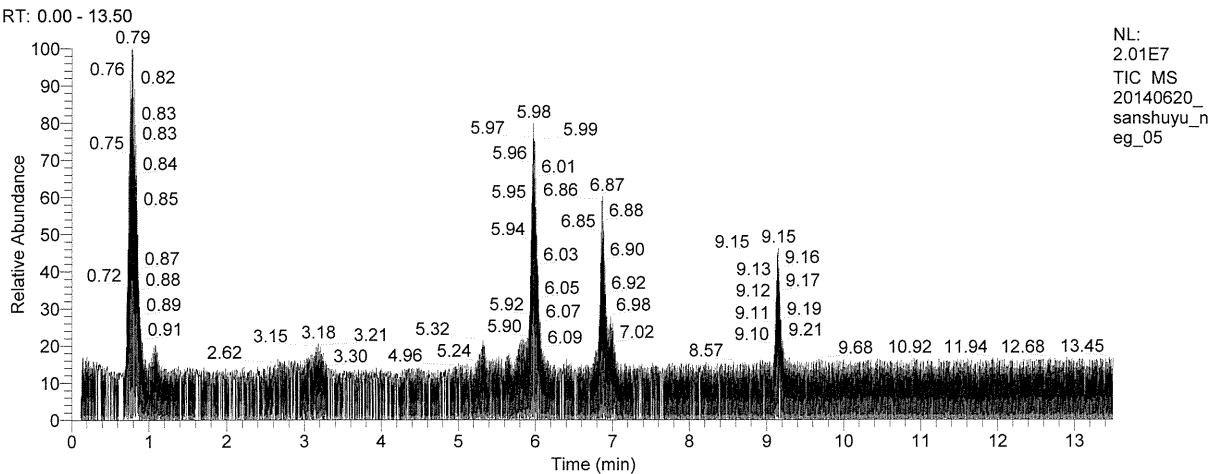
NIB-421



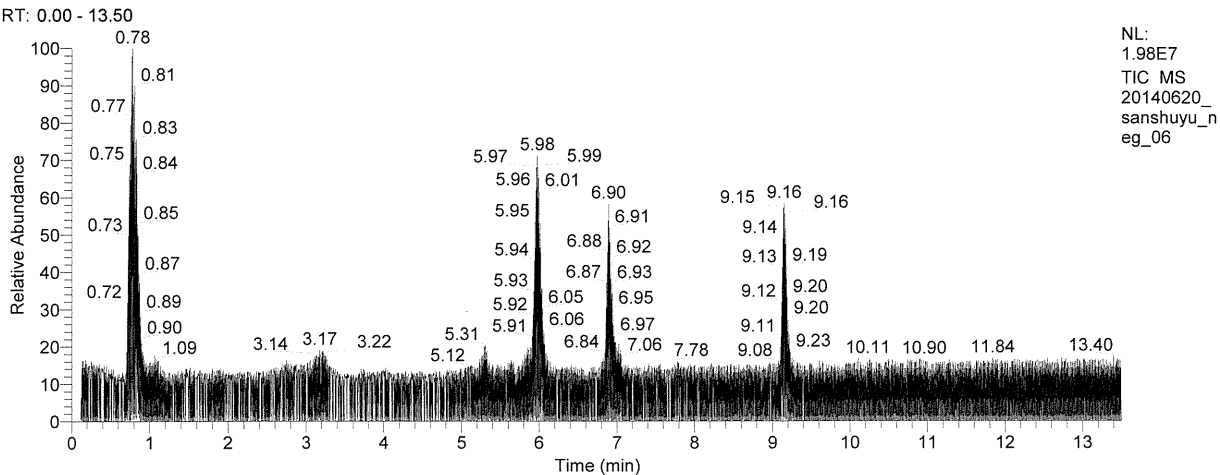
NIB-450



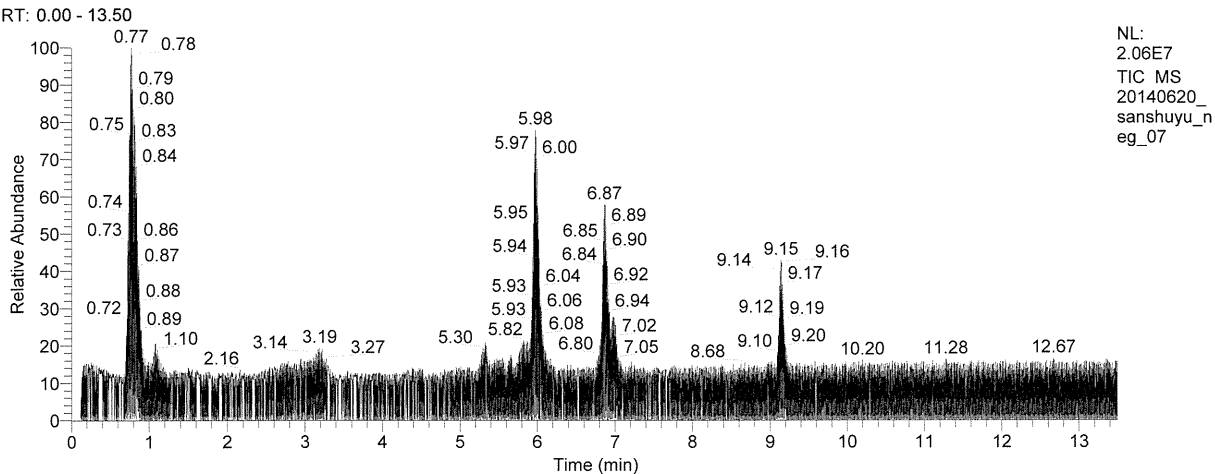
NIB-462



NIB-476

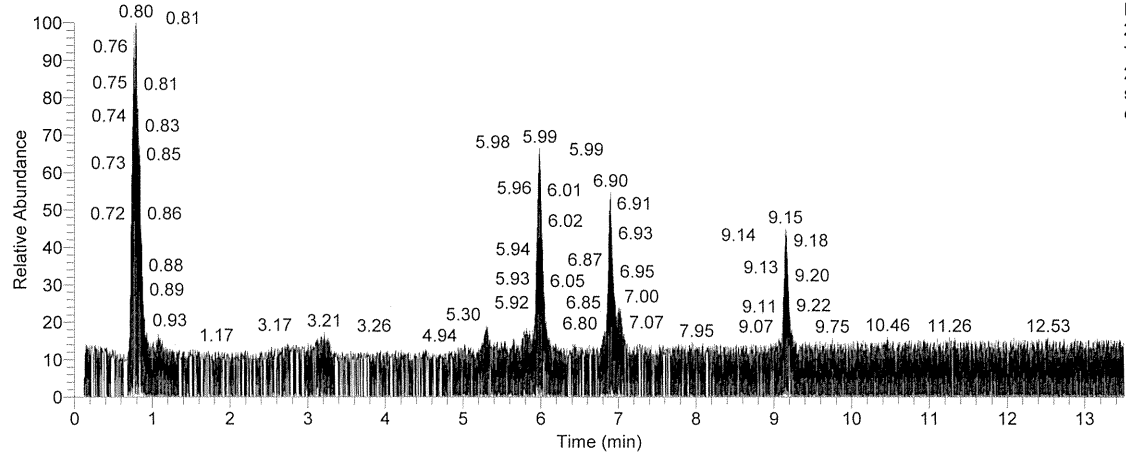


NIB-477



NIB-478

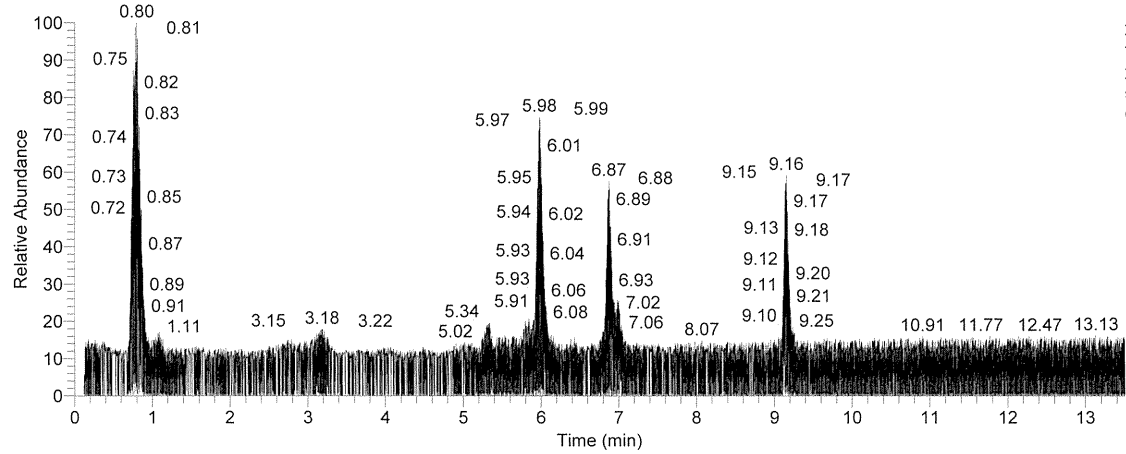
RT: 0.00 - 13.50



NL:
2.09E7
TIC MS
20140620_
sanshuyu_n
eg_08

NIB-479

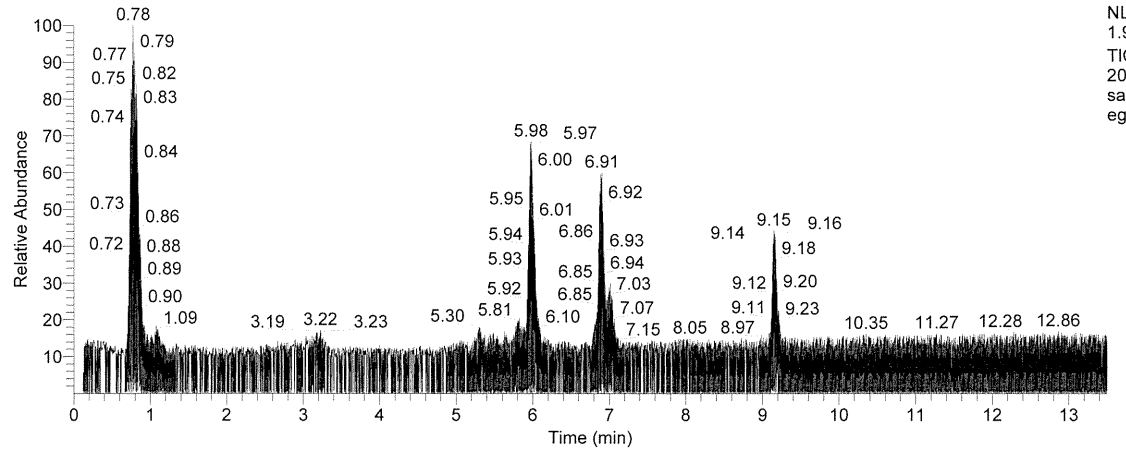
RT: 0.00 - 13.50



NL:
2.03E7
TIC MS
20140620_
sanshuyu_n
eg_09

NIB-480

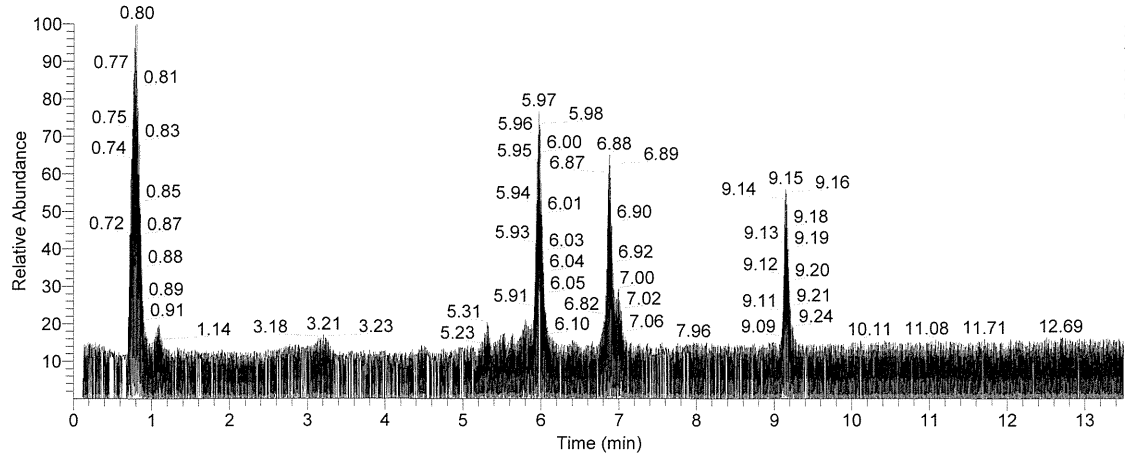
RT: 0.00 - 13.50



NL:
1.99E7
TIC MS
20140620_
sanshuyu_n
eg_10

NIB-481

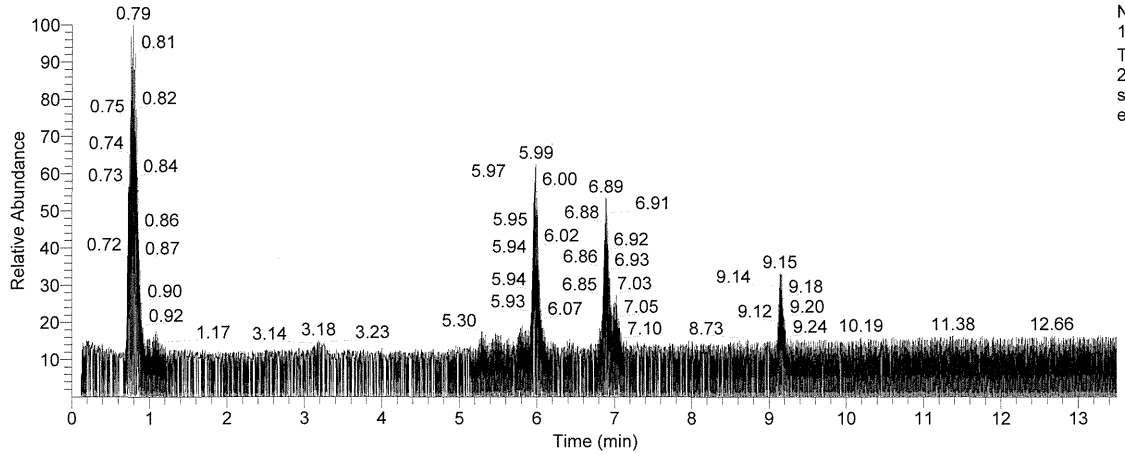
RT: 0.00 - 13.50



NL:
2.02E7
TIC MS
20140620_
sanshuyu_n
eg_11

NIB-482

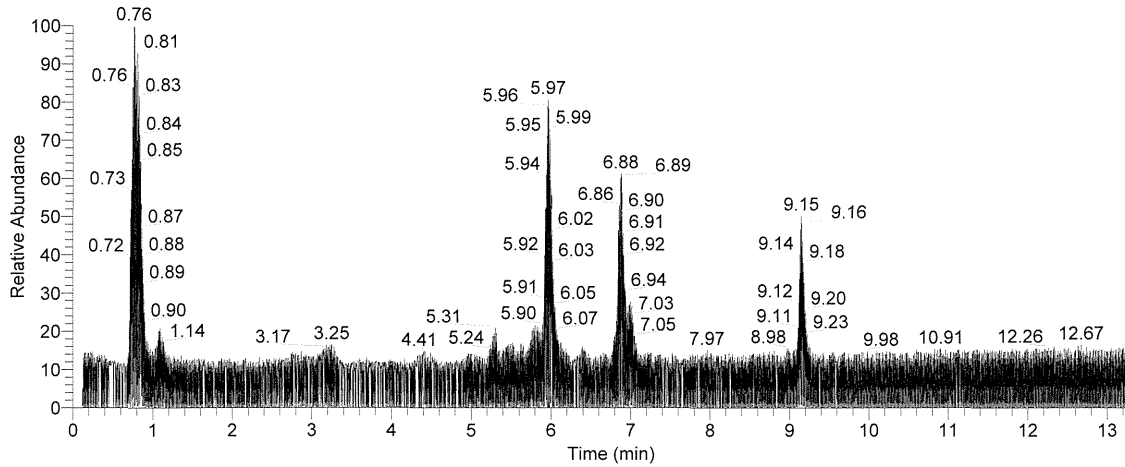
RT: 0.00 - 13.50



NL:
1.97E7
TIC MS
20140620_
sanshuyu_n
eg_12

NIB-483

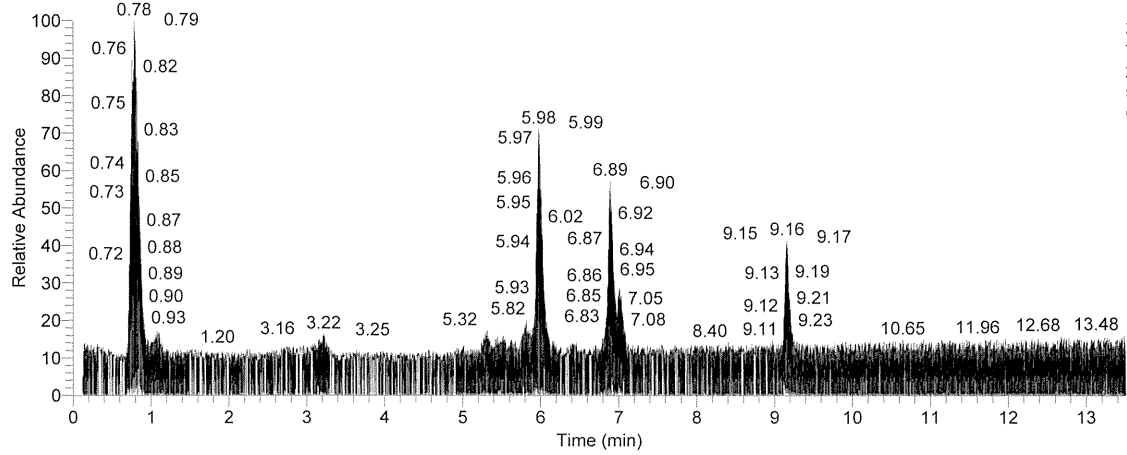
RT: 0.00 - 13.50



NL:
2.06E7
TIC MS
20140620_
Sanshuyu_
Neg_13

NIB-484

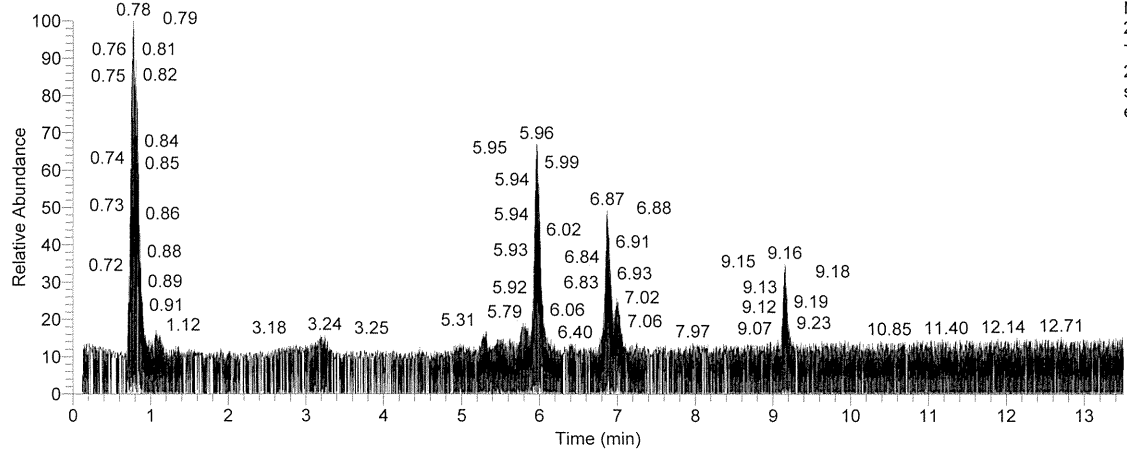
RT: 0.00 - 13.50



NL:
2.14E7
TIC MS
20140620_
sanshuyu_n
eg_14

NIB-485

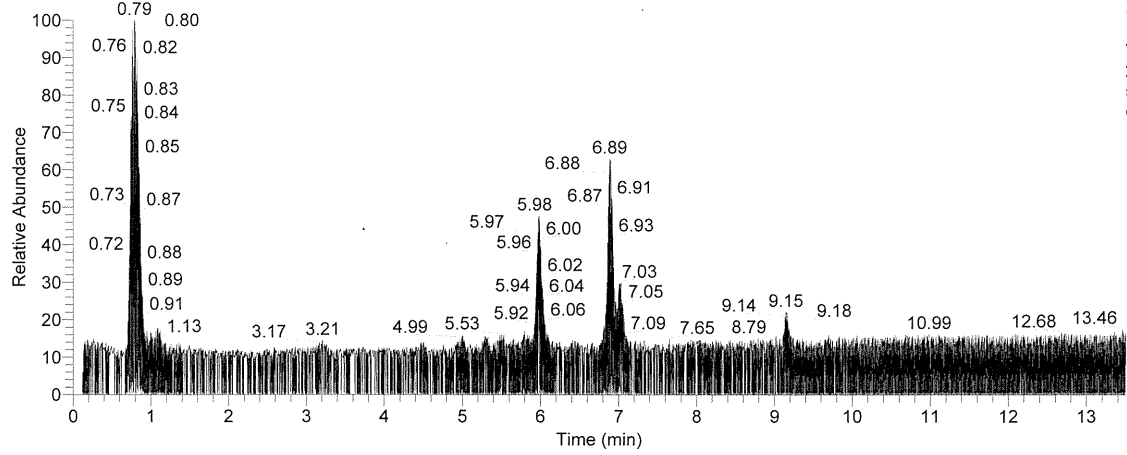
RT: 0.00 - 13.50



NL:
2.17E7
TIC MS
20140620_
sanshuyu_n
eg_15

NIB-486

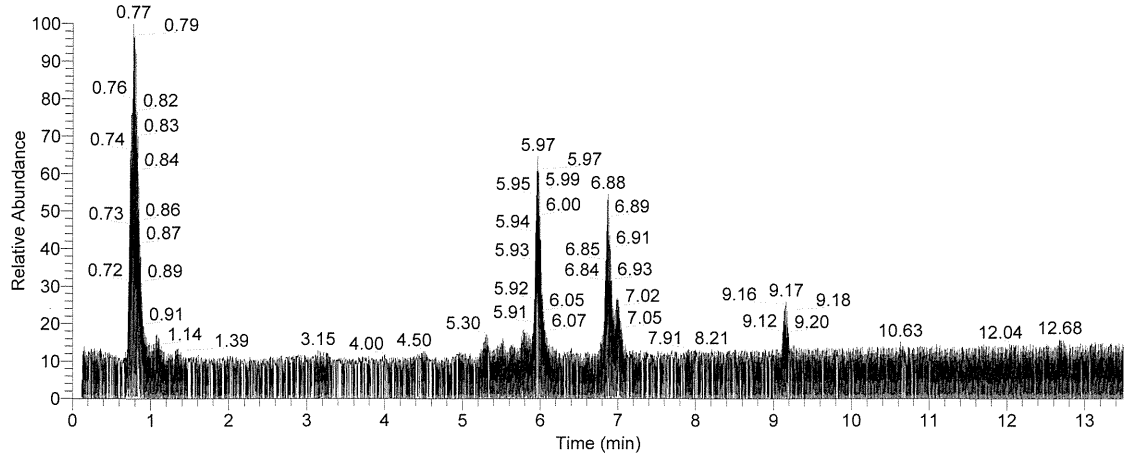
RT: 0.00 - 13.50



NL:
1.97E7
TIC MS
20140620_
sanshuyu_n
eg_16

NIB-487

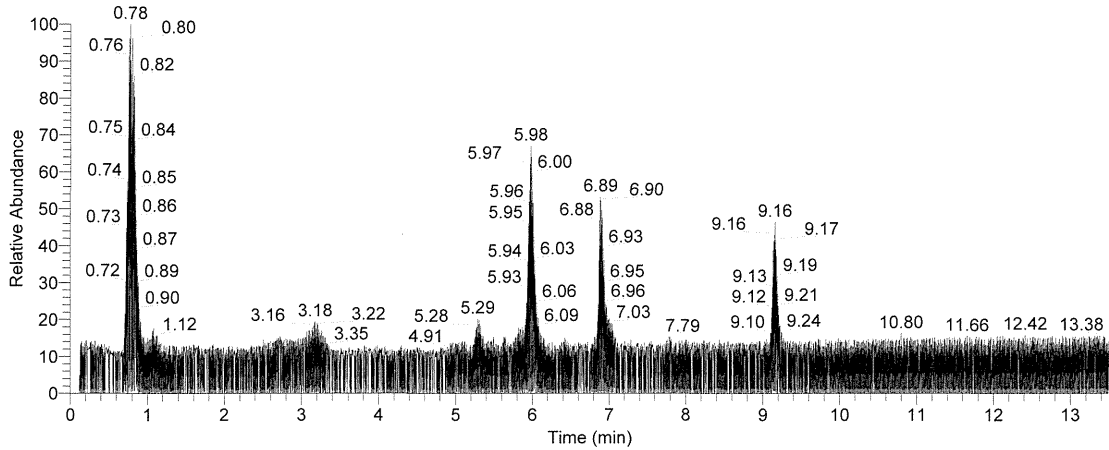
RT: 0.00 - 13.50



NL:
2.20E7
TIC MS
20140620_
sanshuyu_n
eg_17

NIB-648

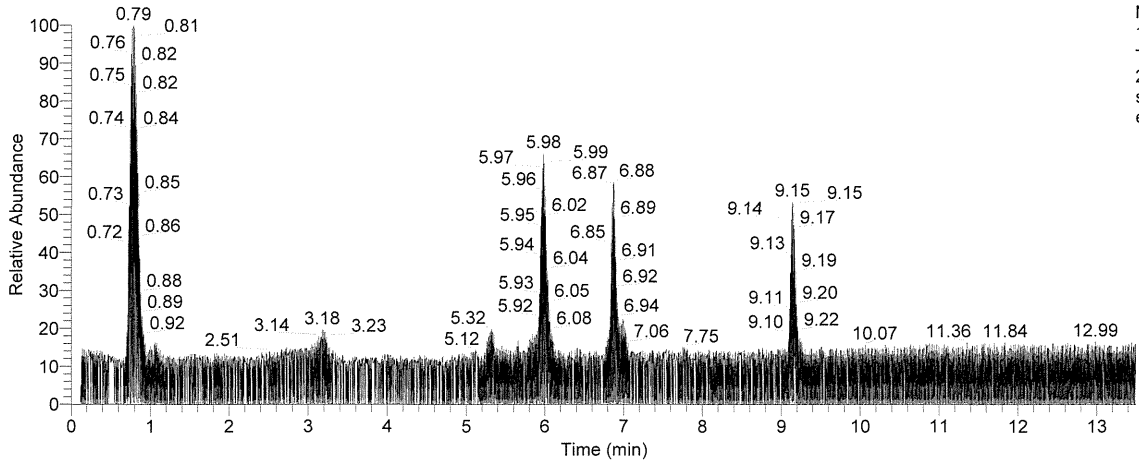
RT: 0.00 - 13.50



NL:
2.03E7
TIC MS
20140620_
sanshuyu_n
eg_18

NIB-741

RT: 0.00 - 13.50



NL:
1.97E7
TIC MS
20140620_
sanshuyu_n
eg_19

サンシュユ 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)
				0.72	149.0091 (1.97E6)	C4H5O6	130.9985(40, C4H3O5), 103.0030(2.56E5; 100, C3H3O4), 87.0083(70, C3H3O3), 59.0140(50,)
				0.76	133.0143 (3.57E6)	C4H5O5 Malic acid	115.0037(1.33E5; 100, C4H3O4)
0.77	219.0268 (5.08E6)		203.1429(3.41E4; 100), 161.0443(10), 129.0031(15)				
	258.1104 (1.92E6)		104.1068(4.07E5; 100)				
				0.78	191.0559 (2.65E6)		
					191.0196 (2.19E6)	C6H7O7	173.0088(15, C6H5O6), 111.0087(5.08E5; 100, C5H3O3)
0.79	335.0381 (1.69E6)		317.0275(60), 275.0365(12), 261.0367(3.61E4; 100), 245.0630(10), 203.0524(12), 173.0207(25)				
0.8	198.0974 (3.13E6)	C6H16O6N	180.0864(15, C6H14O5N), 154.1337(3.45E4; 100), 100.0754(7, C5H10ON), 74.0961(15, C4H12N)				
	180.0867	C6H14O5N	162.0760(30, C6H12O4N), 145.0495(1.50E5; 100, C6H9O4), 127.0388(35, C6H7O3), 97.0281(10, C5H5O2), 85.0281(55, C4H5O2)				
				0.8	295.0672 (8.25E5)	C10H15O10	277.0566(20, C10H13O9), 235.0459(40, C8H11O8), 205.0353(15, C7H9O7), 179.0559(1.95E5; 100, C6H11O6), 161.0455(15, C6H9O5), 143.0350(13, C6H7O4), 133.0143(70, C4H5O5), 119.0351(12,), 101.0245(10)
					353.0726 (7.95E5)	C12H17O12	173.0089(65, C6H5O6), 111.0087(1.07E5; 100, C5H3O3)
				0.87	169.0141 (7.01E5)	C7H5O5 Gallic acid or Isomer	125.0243(2.29E5; 100, C6H5O3)
				1.08	169.0138 (9.82E5)	C7H5O5 Gallic acid or Isomer	125.0243(4.73E5; 100, C6H5O3)
4.36	268.1038 (5.93E4)	C10H14O4N5	136.0616(1.33E5; 100, C5H6N5)				
4.42	334.1494 (5.66E4)	C14H24O8N ([M+NH4])	289.0918(60, C12H17O8), 271.0811(75, C12H15O7), 253.0706(15, C12H13O6), 137.0596(6.21E3; 100, C8H9O2), 127.0389(50, C6H7O3)				
				4.48	483.0763 (3.98E5)	C20H19O14	331.0662(1.52E5; 100, C13H15O10), 313.0557(25, C13H13O9), 169.0137(25, C7H5O5)
5.32	394.1705 (1.97E5)	C16H28O10N ([M+NH4])	377.1434(20, C16H25O10: [M+H]+), 359.1329(10, C16H23O9),	5.31	375.1286 (8.78E5)	C16H23O10	213.0761(4.40E4; 100, C10H13O5:

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)
			341.1222(15, C16H21O8), 215.0909(1.86E4; 100, C10H15O5: MH-Glc), 197.0805(10, C10H13O4), 179.0699(7, C10H11O3)				-Glc), 169.0864(20, C9H13O3)
5.43	586.2328 (1.05E5)	C23H40O16N	551.1958(13, C23H35O15), 406.1697(7, C17H28O10N), 389.1432(15, C17H25O10), 227.0909(5.78E4; 100, C11H15O5), 209.0804(10, C11H13O4), 195.0648(25, C10H11O4), 183.0648(10, C9H11O4)				
	614.2640 (5.26E4)	C25H44O16N	596.2529(5, C25H42O15N), 434.2007(95, C19H32O10N), 389.1428(5, C17H25O10), 227.0908(1.64E4; 100, C11H15O5), 209.0803(12, C11H13O4), 195.0648(35, C10H11O4), 183.0647(10, C9H11O4)				
				5.49	509.1287 (2.89E5)	C23H25O13	385.0759(8, C16H17O11), 329.0652(8.01E4; 100, C17H13O7: -Glc(+OH)), 285.0757(25, C16H13O5), 270.0524(10, C15H10O5), 205.0133(30, C10H5O5)
				5.53	491.1393 (3.08E5)	C20H27O14	473.1288(8, C20H25O13), 375.1287(1.54E5; 100, C16H23O10), 213.0762(10, C10H13O5)
5.63	586.2328 (8.72E4)	C23H40O16N	551.1958(13, C23H35O15), 406.1694(5, C17H28O10N), 389.1429(15, C17H25O10), 227.0907(4.22E4; 100, C11H15O5), 209.0802(10, C11H13O4), 195.0647(30, C10H11O4), 183.0647(10, C9H11O4)				
	227.0911	C11H15O5	209.0809(8, C11H13O4), 195.0653(4.24E4; 100, C10H11O4), 177.0546(5, C10H9O3), 141.0546(50, C7H9O3)				
5.64	424.1805 (1.37E6)	C17H30O11N ([M+NH4])		5.64	451.1447 (1.84E5)	C18H27O13 ([M+HCOO]-)	405.1390(1.04E5;100, C17H25O11: [M-H]-), 243.0868(15, C11H15O6: M-H-Glc), 179.0554(3, C6H11O6)
5.79	540.1922 (9.64E4)	C21H34O15N ([M+NH4])	522.1365(20), 505.1537(1.73E4; 100, C21H29O14), 487.1433(40, C21H27O13), 469.1330(15, C21H25O12), 279.0702(50, C21H25O12), 261.0597(25, C10H13O8), 227.0908(80, C11H15O5), 209.0803(25, C11H13O4), 181.0855(10, C13H9O)	5.79	521.1490 (5.96E5)	C21H29O15 ([M-H]-)	503.1391(35, C21H27O14), 445.1339(13, C19H25O12), 347.1339(7, C15H23O9), 243.0869(85, C11H15O6), 179.0554(20, C6H11O6)
5.81	422.1956 (1.57E5)	C17H28O11N ([M+NH4])	405.1388(1.58E3; 100, C17H25O11), 243.0860(40, C11H15O6), 229.1066(20, C11H17O5), 211.0959(17, C11H15O4), 167.0701(20, C9H11O3)				

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)
	405.139	C17H25O11 ([M+H] ⁺)	243.0861(1.69E4; 100, C11H15O6), 211.0600(60, C11H15O4), 167.0337(12, C9H11O3)				
	450.1969 (2.94E5)	C19H32O11N	405.1379(45), 243.0855(7.30E4; 100), 211.0596(60), 167.0334(15)				
5.89	598.2336 (7.55E4)	C24H40O16N ([M+NH4] ⁺)	563.1953(4.39E4; 100, C24H35O15), 545.1849(7, C24H33O14), 337.1119(45, C13H21O10), 319.1013(15, C13H19O9), 227.0908(7, C11H15O5), 209.0802(25, C11H13O4), 181.0854(15, C10H13O3)				
				5.93	513.0873 (7.00E5)	C21H21O15	423.0556(10, C18H15O12), 361.0766(20, C14H17O11), 343.0661(12, C14H15O10), 271.0453(1.00E5; 100, C11H11O8), 241.0346(8, C10H9O7), 211.0241(20, C9H7O6), 169.0136(25, C7H5O5)
5.97	424.1805 (6.37E6)	C17H30O11N ([M+NH4] ⁺) Morrisoniside	406.1703(25, C17H28O10N), 389.1436(15, C17H25O10), 227.0912(5.56E5; 100, C11H15O5), 209.0809(2, C11H13O4), 195.0650(10, C10H11O4)	5.97	451.1444 (5.43E6)	C18H27O13 ([M+HCOO] ⁻) Morrisoniside	405.1389(3.95E6;100, C17H25O11: [M-H] ⁻), 243.0869(20, C11H15O6), 179.0555(15, C6H11O6)
	406.1704	C17H28O10N	389.1430(8, C17H25O10), 388.1589(10, C17H26O9N), 244.1171(5, C11H18O5N), 227.0907(2.35E5; 100, C11H15O5), 209.0802(10, C11H13O4), 195.0646(20, C10H11O4), 183.0646(10, C9H11O4), 140.0701(2, C7H10O2N)		405.1394	C17H25O11 ([M-H] ⁻) Morrisoniside	373.1132(30, C16H21O10), 243.0868(9.93E3; 100, C11H15O6), 225.0760(13, C11H13O5), 179.0554(30, C6H11O6), 155.0344(20, C7H7O4), 141.0553(15, C7H9O3)
	429.1357	C17H26O11Na	411.1253(35), 385.1099(20), 383.1304(15), 341.0170(7), 313.0888(10), 273.0938(75), 271.0782(60), 267.0833(1.82E5; 100), 255.0833(25), 249.0727(15), 235.0571(17), 223.0573(13), 203.0523(15), 185.0417(30), 181.0467(20), 179.0311(15)				
	227.0911	C11H15O5	209.0807(30, C11H13O4), 195.0651(5.53E5; 100, C10H11O4), 183.0650(35, C9H11O4), 181.0494(15, C9H9O4), 177.0545(7, C10H9O3), 167.0702(7, C9H11O3), 141.0545(12, C7H9O3), 127.0388(5, C6H7O3)				
6.03	540.1926 (8.47E4)	C21H34O15N ([M+NH4] ⁺)	522.1791(20), 505.1537(1.73E4; 100, C21H29O14), 487.1433(40, C21H27O13), 469.1330(15, C21H25O12), 279.0702(50, C21H25O12), 261.0597(25, C10H13O8), 227.0908(80, C11H15O5), 209.0803(25, C11H13O4), 181.0855(10, C13H9O)				
6.4	441.1728 (1.23E5)	C19H30O10Na ([M+Na] ⁺)	426.1485(35, C18H27O10Na), 411.1613(12, C18H28O9Na), 279.1194(1.02E4; 100, C13H20O5Na:				

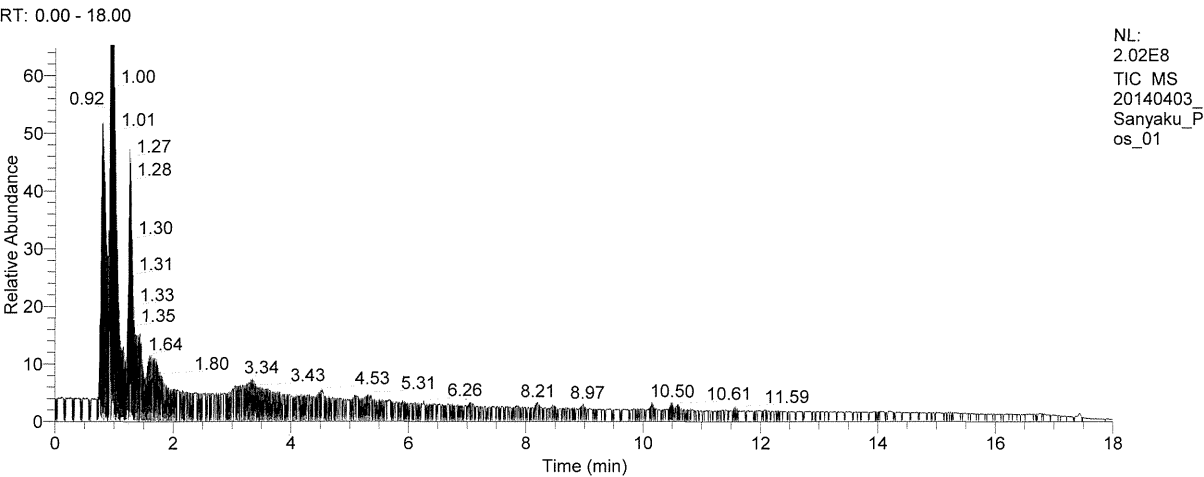
正イオン検出				負イオン検出			
RT	m/z(強度)	推定組成	プロダクトイオン(強度)	RT	m/z(強度)	推定組成	プロダクトイオン(強度)
			-Glc), 259.0779(65, C9H16O7Na), 247.0935(10, C12H16O4Na), 203.0522(25, C6H12O6Na), 201.0364(10, C6H10O6Na)				
	436.2172	C19H34O10N ([M+NH4])	405.1384(15), 391.2835(25), 257.1378(9.18E3; 100, C13H21O5, MH-Glc), 243.0858(15, C11H15O6), 229.1066(80, C11H17O5), 211.0962(20, C11H15O4)				
6.81	392.1913 (5.94E4)	C17H30O9N ([M+NH4])	213.1119(9.71E4; 100, C11H17O4: MH-Glc), 195.1013(5, C11H15O3), 167.0700(5, C9H11O3), 149.0231(8, C8H5O3)				
6.87	524.1971 (2.27E5)	C21H34O14N ([M+NH4]+)	507.1694(60, C21H31O14: [M+H]+), 489.1588(2.39E4; 100, C21H29O13), 471.1484(80, C21H27O12), 457.1327(40, C20H25O12), 453.1379(20, C21H25O11), 209.0804(15, C11H13O4)	6.83	505.1542 (1.38E6)	C21H29O14	487.1444(5.87E4; 100, C21H27O13), 389.1445(25, C17H25O10), 227.0919(85, C11H15O5: 389-Glc)
6.89	408.1865 (3.54E6)	C17H30O10N ([M+NH4]+) Loganin	229.1064(8.66E3; 100, C11H17O5: MH-Glc)	6.88	435.1494 (4.80E6)	[M+HCOO]- Loganin	389.1443(25, C17H25O10: [M-H]-), 227.0919(1.74E4; 100, C11H15O5: M-H-Glc)
	229.1071	C11H17O5	211.0964(25, C11H15O4), 197.0808(30, C10H13O4), 193.0859(12, C11H13O3), 179.0702(3.86E5; 100, C10H11O3), 161.0597(5, C10H9O2), 151.0753(8, C9H11O2), 119.0338(15, C4H7O4), 109.0646(30, C7H9O), 81.0696(8, C6H9)				
6.95	404.1913 (3.15E5)	C18H30O9N	359.1331(2.82E5; 100, C16H23O9), 197.0807(20, C10H13O4: 359-Glc)				
	359.1333 (1.29E6)	C16H23O9 ([M+H]+) Sweroside	197.0808(2.08E5; 100, C10H13O4: -Glc), 179.0702(10, C10H11O3), 127.0388(8, C6H7O3)	6.93	403.1235 (5.70E5)	C17H23O11 ([M+HCOO]-) Sweroside	357.1177(4.65E4; 100, C16H21O9: [M-H]-), 195.0655(45, C10H11O4: M-H-Glc), 179.0554(40, C6H11O6), 161.0450(13, C6H9O5), 125.0241(35, C6H5O3)
	197.0808	C10H13O4	179.0701(2.65E5; 100, C10H11O3), 161.0596(10, C10H9O2), 151.0753(45, C9H11O2), 137.0596(20, C8H9O2), 127.0388(40, C6H7O3), 109.0646(30, C7H9O)				
7.01	524.1977 (2.60E5)	C21H34O14N ([M+NH4]+)	489.1588(10, C21H29O13), 345.1172(4.54E4; 100, C15H21O9: MH-Glc), 327.1069(13, C15H19O8), 211.0961(40, C11H15O4), 193.0856(25, C11H13O3), 179.0698(7, C10H11O3)	7	505.1548 (1.65E6)	C21H29O14 ([M-H]-)	487.1438(80, C21H27O13), 389.1440(25, C17H25O10), 227.0918(4.21E5; 100, C11H15O5: 389-Glc)
7.05	582.2377 (8.97E4)	C24H40O15N ([M+NH4])	403.1593(12, C18H27O10: MH-Glc), 211.0962(3.52E4; 100, C11H15O4), 193.0856(50, C11H13O3), 179.0700(20, C10H11O3)				
8.99	350.2173 (5.91E4)	C16H32O7N ([M+NH4])					
	355.1727	C16H28O7Na ([M+Na]+)	203.0523(6.50E3; 100, C6H12O6Na), 193.1197(40, C10H18O2Na: -Glc)				
9.15	560.1973 (7.27E5)	C24H34O14N ([M+NH4]+)	381.1171(70, C18H21O9: MH-Glc), 373.1485(20, C18H19O8), 349.0913(8,	9.16	541.1547 (5.50E6)	C24H29O14 ([M-H]-)	379.1024(45, C18H19O9: -Glc),

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)
			C17H17O8), 211.0962(2.47E4; 100, C11H15O4)				347.0763(90, C17H15O8), 309.0608(15, C14H13O8), 277.0712(20, C14H13O6), 195.0657(10, C10H11O4), 169.0137(1.15E5; 100, C7H5O5)
	211.0965	C11H15O4	193.0861(5, C11H13O3), 179.0704(30, C10H11O3), 151.0754(10, C9H11O2), 141.0547(1.48E5; 100, C7H9O3)				
9.24	531.2328 (5.06E4)	C27H35O9N2 ([M+NH4]+)	514.2059(8.97E4; 100, C27H32O9N: [M+H]+), 369.1799(20, C21H25O4N2: -Glc), 352.1537(10, C21H22O4N: MH-Glc)				
9.27	532.2026 (3.74E4)	C23H34O13N ([M+NH4]+)					
	251.1753 (5.60E4)	C14H23O2N2	233.1647(9.65E4; 100, C14H21ON2)				

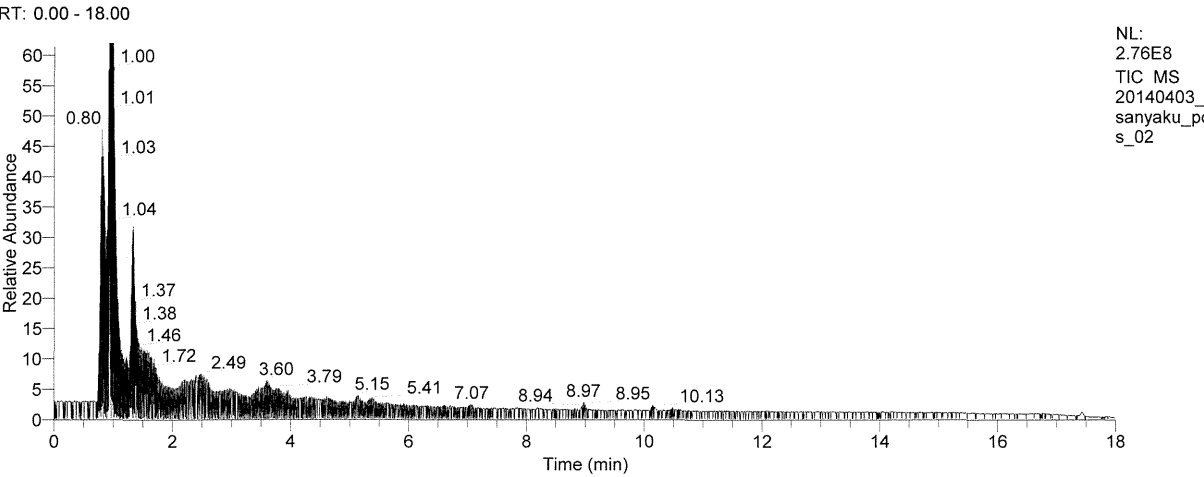
サンヤク LC/MS データ (positive mode)

TIC

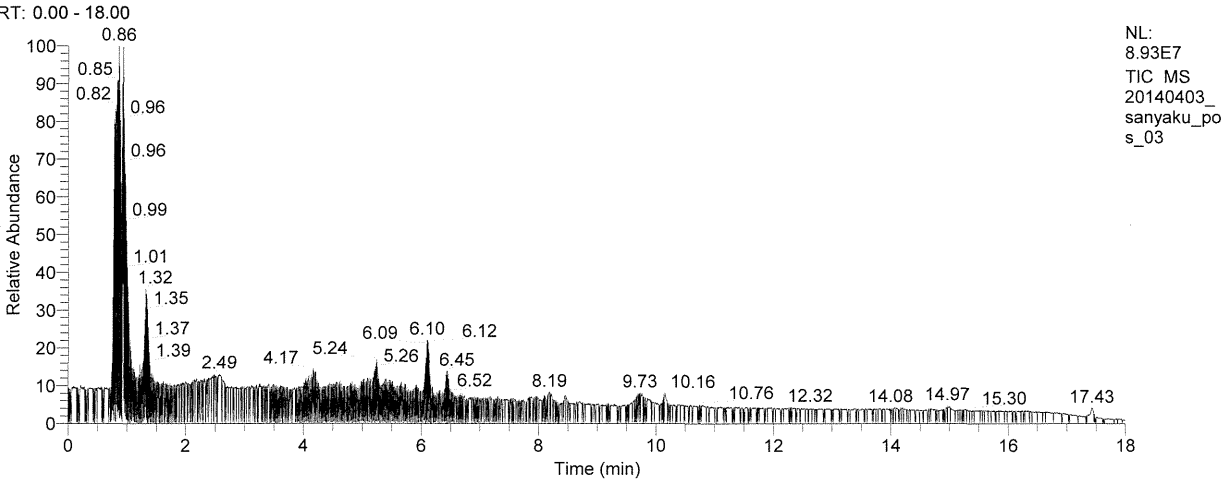
NIB-255_Pos



NIB-401_Pos

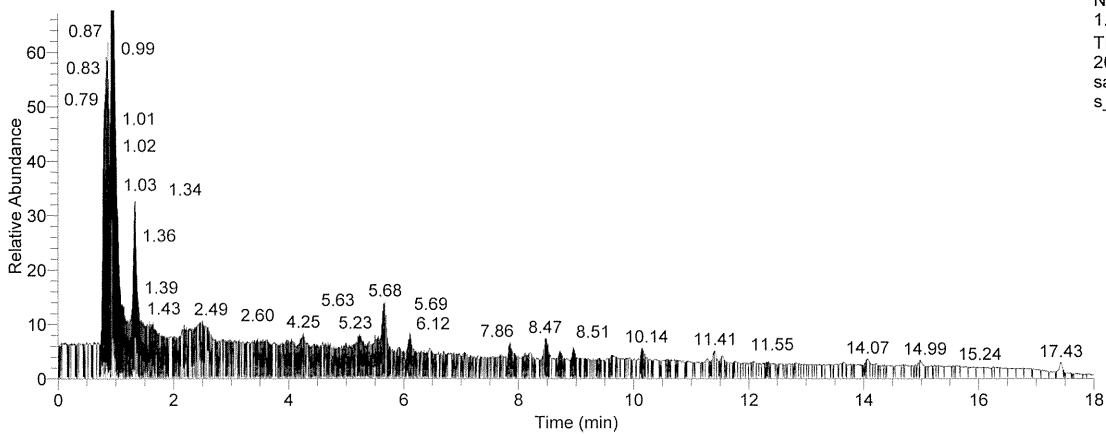


NIB-456_Pos



NIB-566_Pos

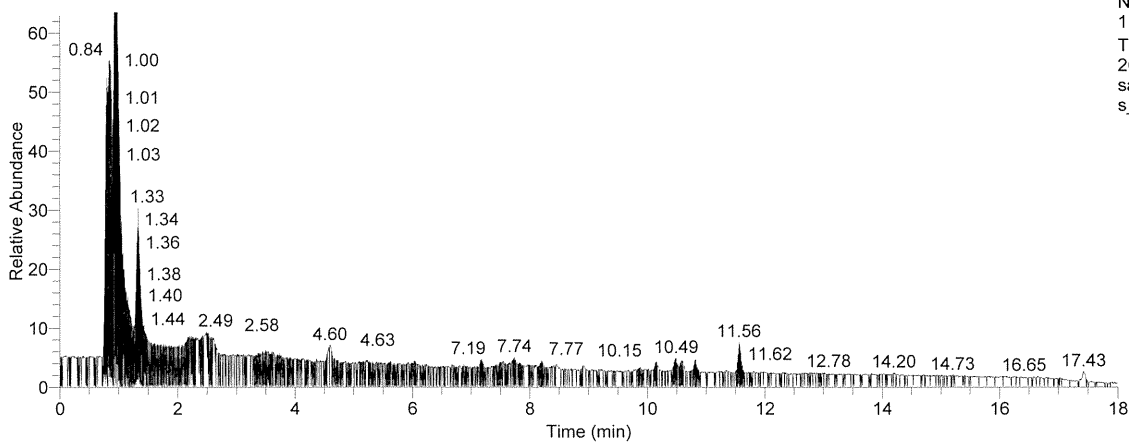
RT: 0.00 - 18.00



NL:
1.30E8
TIC MS
20140403_
sanyaku_po
s_04

NIB-567_Pos

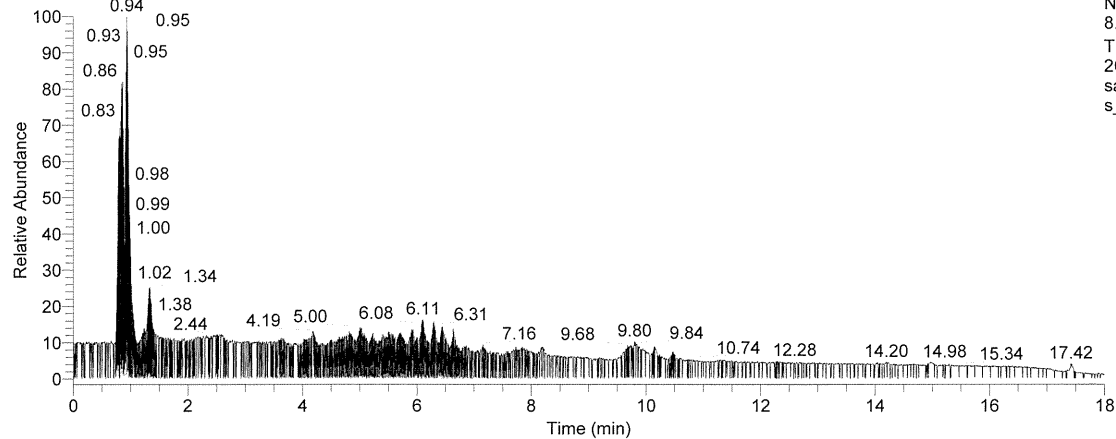
RT: 0.00 - 18.00



NL:
1.59E8
TIC MS
20140403_
sanyaku_po
s_05

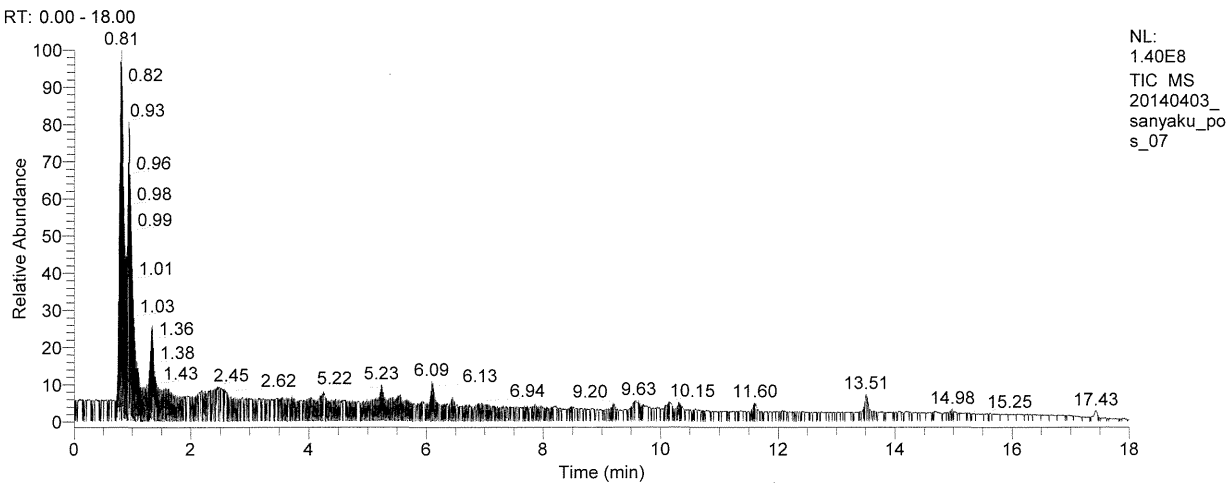
NIB-568_Pos

RT: 0.00 - 18.00



NL:
8.21E7
TIC MS
20140403_
sanyaku_po
s_06

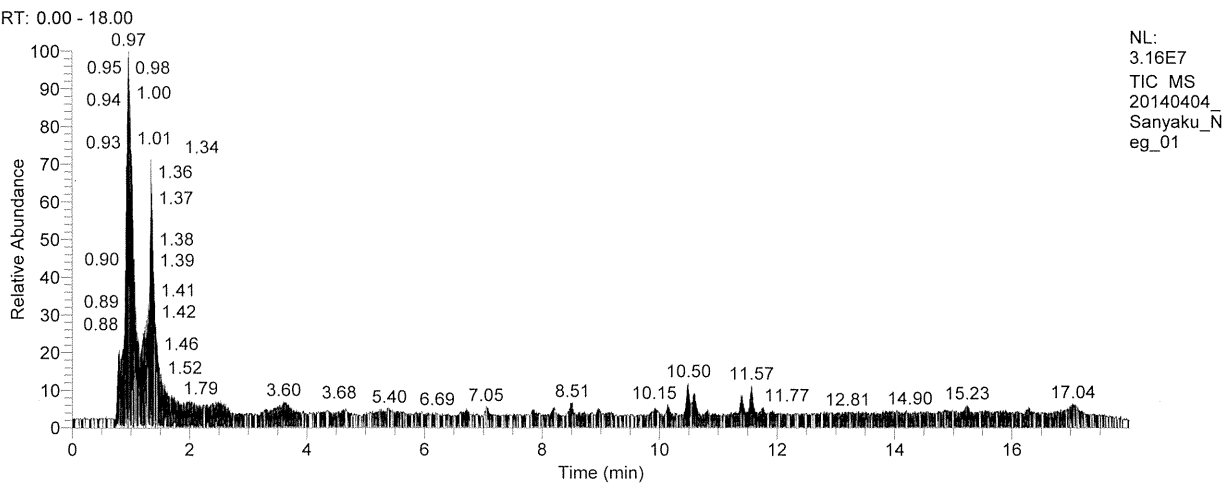
NIB-748_Pos



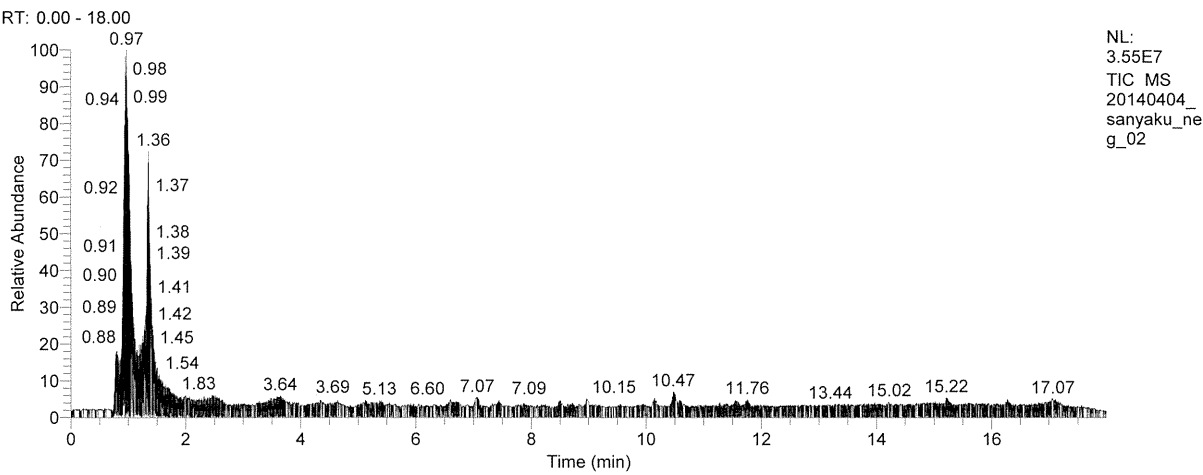
サンヤク LC/MS データ (negative mode)

TIC

NIB-255_Neg



NIB-401_Neg



NIB-456_Neg

