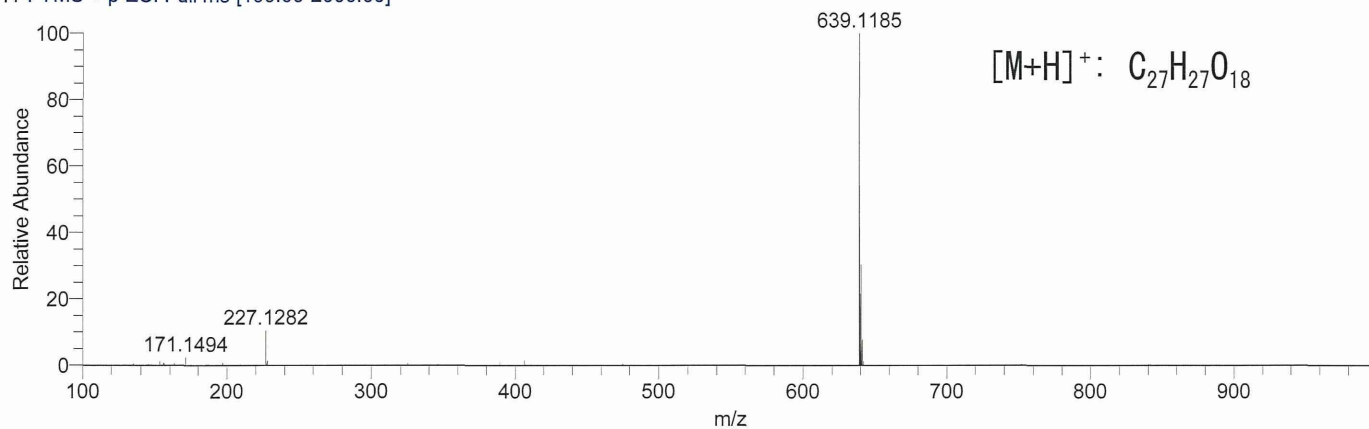


図 16 ソヨウ (NIB-200) のポジティブイオンモードにおける TIC (上段) 及びネガティブモードにおける TIC (下段)

20120517_Soyo-Pos_04 #816 RT: 12.58 AV: 1 NL: 4.40E7
T: FTMS + p ESI Full ms [100.00-2000.00]



20120517_Soyo-Pos_04 #827 RT: 12.75 AV: 1 NL: 8.31E6
T: FTMS + p ESI d Full ms2 639.12@cid35.00 [165.00-650.00]

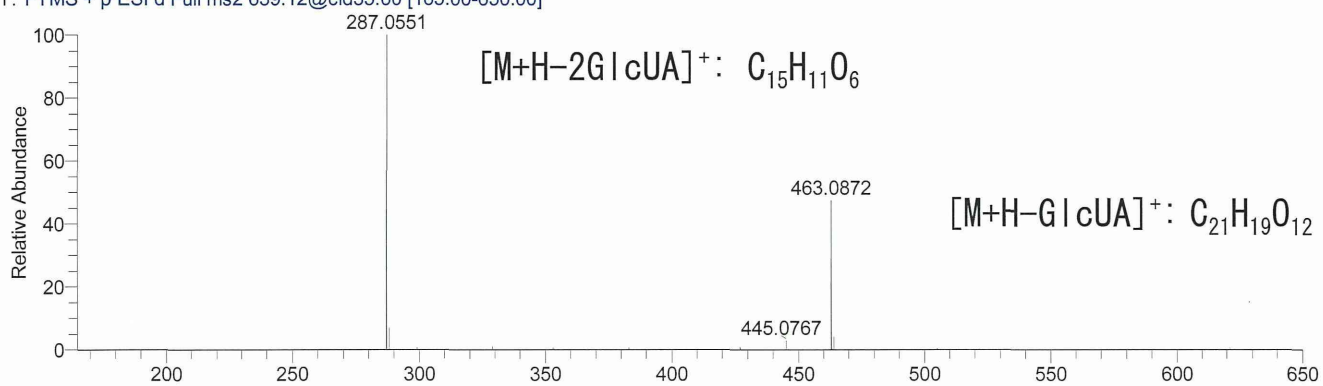
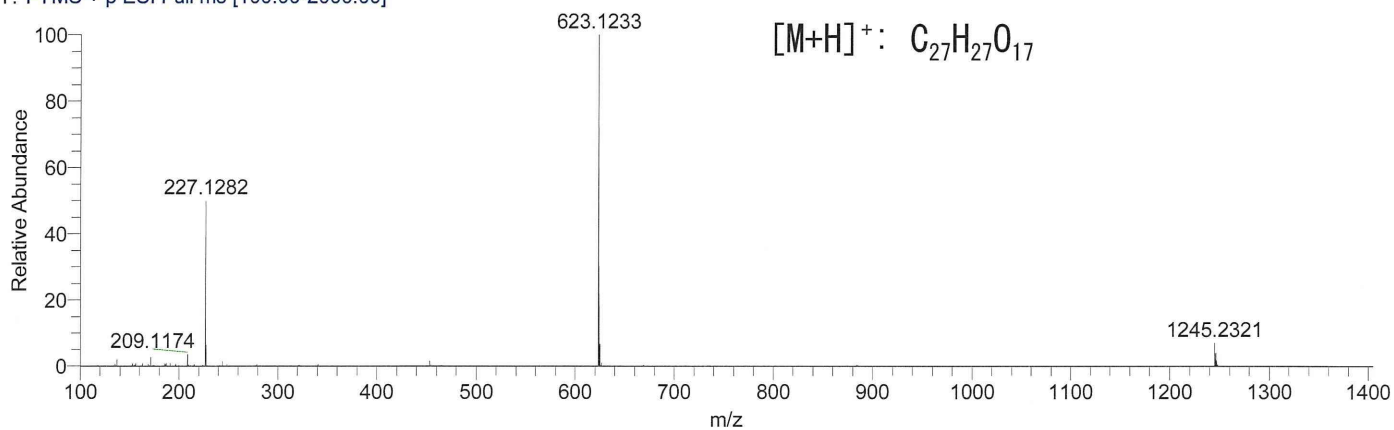


図 17 Peak 1 のポジティブモードでの MS (上段) 及び MS/MS (下段)

20120517_Soyo-Pos_04 #898 RT: 13.83 AV: 1 NL: 3.68E7
T: FTMS + p ESI Full ms [100.00-2000.00]



20120517_Soyo-Pos_04 #893 RT: 13.76 AV: 1 NL: 6.21E6
T: FTMS + p ESI d Full ms2 623.12@cid35.00 [160.00-635.00]

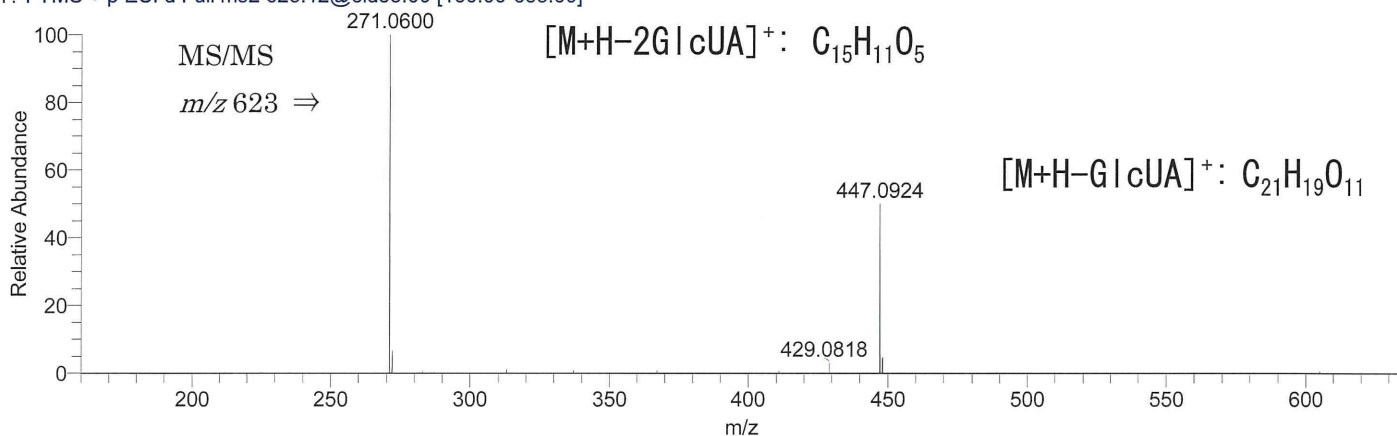
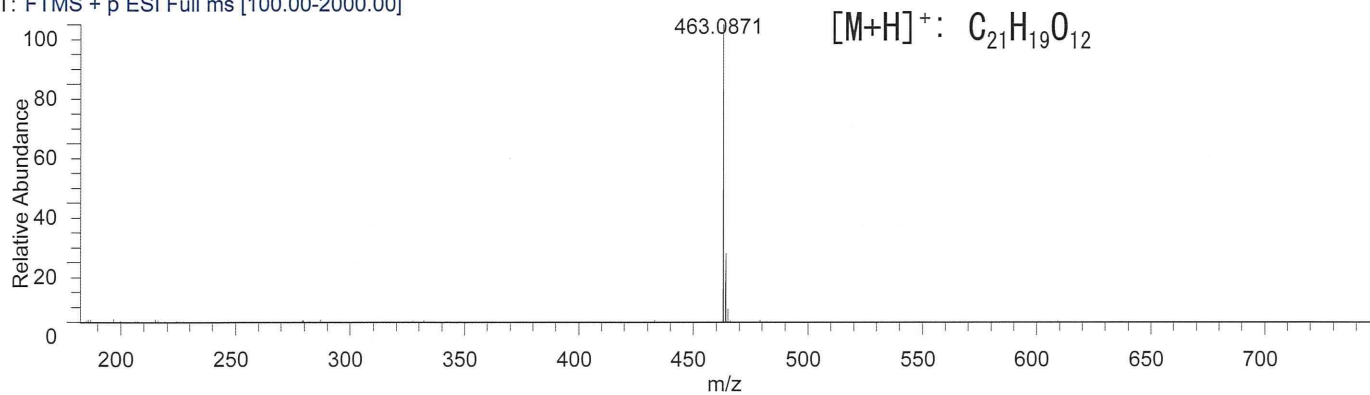


図 18 Peak 2 のポジティブモードでの MS (上段) 及び MS/MS (下段)

20120517_Soyo-Pos_04#966 RT: 14.86 AV: 1 NL: 3.15E7
T: FTMS + p ESI Full ms [100.00-2000.00]



20120517_Soyo-Pos_04 #961 RT: 14.78 AV: 1 NL: 5.06E6
T: FTMS + p ESI d Full ms2 463.09@cid35.00 [115.00-475.00]

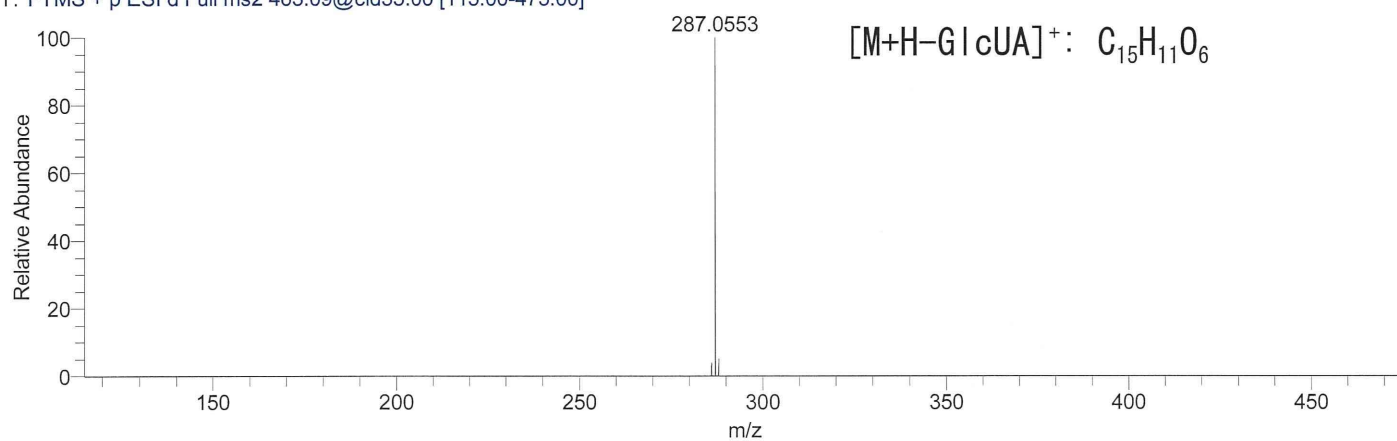
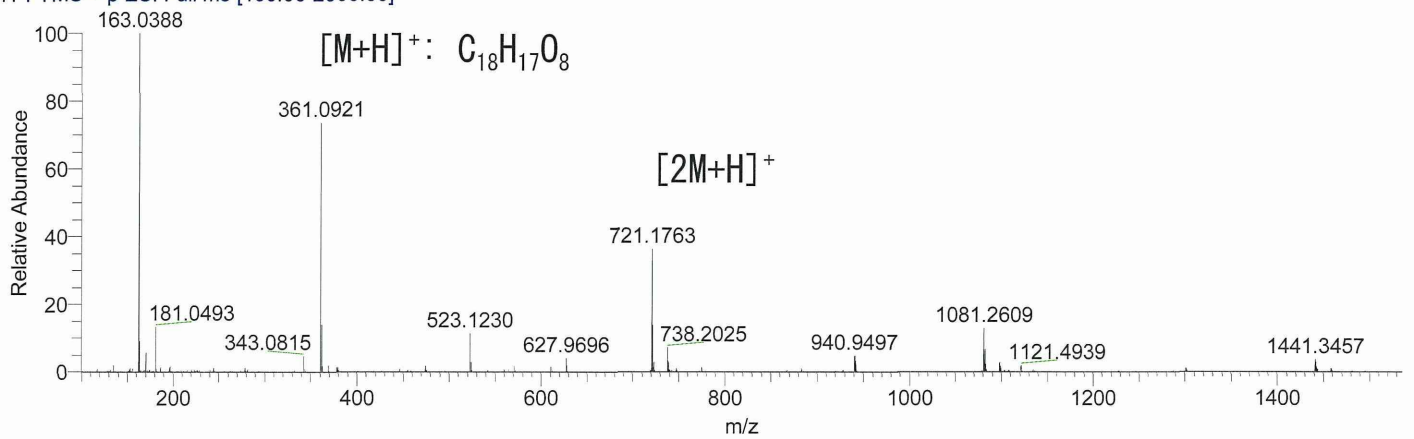


図 19 Peak 3 のポジティブモードでの MS (上段) 及び MS/MS (下段)

20120517_Soyo-Pos_04 #1086 RT: 16.71 AV: 1 NL: 1.69E7
T: FTMS + p ESI Full ms [100.00-2000.00]



20120517_Soyo-Pos_04 #1079 RT: 16.60 AV: 1 NL: 1.35E6
T: FTMS + p ESI d Full ms2 361.09@cid35.00 [85.00-375.00]

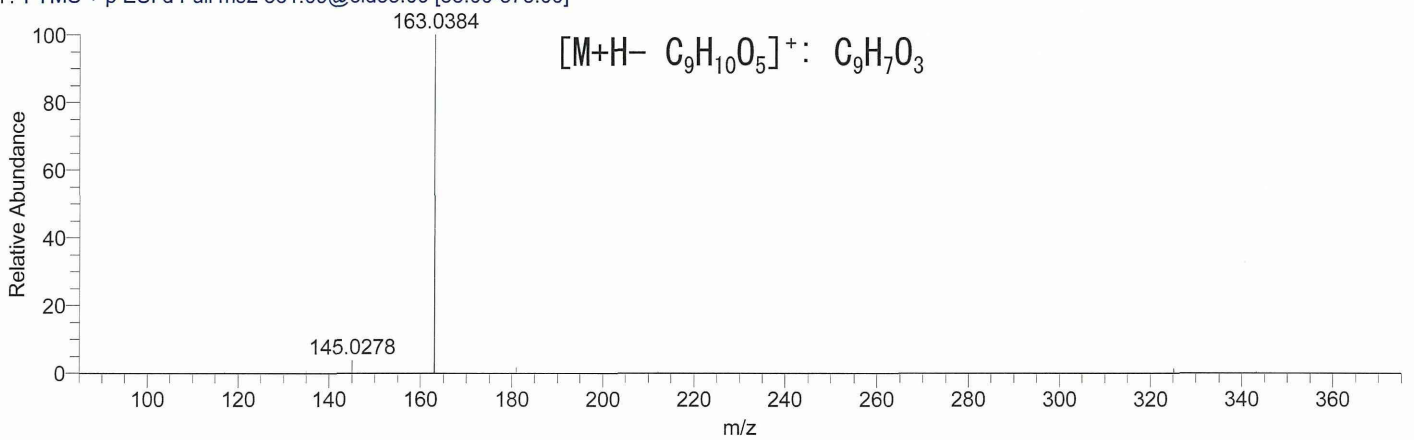


図 20 Peak 4 のポジティブモードでの MS (上段) 及び MS/MS (下段)

表1 ダイオウスペクトルリスト(Pos_1)

保持時間 (min)	m/z	推定組成	プロダクトイオン
1.91	184.0455		161.0289(20), 143.0183(7.67E6; 100), 124.0238(70), 101.0080(10)
2.16	175.1192	C6H15O2N4	175(70), 158.0921(1.07E6; 100), 130.0972(40), 116.0704(50)
2.25	458.1863	C17H32O13N	398.0458(3.78E5; 100)
2.5	360.1508 343+NH3	C12H26O11N	343.1237(20, C12H23O11), 325.1133(1.13E6; 100, C12H21O10), 307.1025(10, C12H19O9), 289.0919(30, C12H17O8), 259.0811(20, C11H15O7), 163.0596(30, C6H11O5), 145.0490(25, C6H9O4), 127.0384(20,)
3.32	182.0817	C9H12O3N	182(15), 165.0543(7.23E6; 100, C9H9O3), 147.0436(5, C9H7O2), 136.0752(30,)
3.5	132.102	C6H14O2N	86.0961 (2.32E6; 100, C5H12N)
4.32	166.0864	C9H12O2N	120.0804(2.71E6; 100, C8H10N)
5.34	453.1391	C21H25O11	435.1285(5, C21H23O10), 417.1180(5, C21H21O9), 301.0916(20, C13H17O8), 291.0862(6.55E5; 100, C15H15O6), 273.0754(5, C15H13O5)
6.8-7.5	205.0978	C11H13O2N2	188.0708(7.88E6; 100, C11H10O2N), 163.0180(10,), 145.0073(5,)
7.6-8.1	122.0967	C8H12N	105.0696(1.68E7; 100, C8H9)
8.39	453.139	C21H25O11	435.1284(10, C21H23O10), 417.1178(10, C21H21O9), 315.0861(5, C17H15O6), 301.0914(20, C13H17O8), 291.0861(1.25E6; 100, C15H15O6), 273.0753(10, C15H13O5)
8.58	579.1493	C30H27O12	561.1395(5, C30H25O11), 453.1178(5, C24H21O9), 427.1024(1.17E6; 100, C22H19O9), 409.0919(70, C22H17O8), 301.0704(20, C16H13O6), 291.0861(50, C15H15O6), 271.0599(10, C15H11O5), 247.0597(20, C13H11O5)
8.78	579.1488	C30H27O12	561.1393(15, C30H25O11), 453.1178(10, C24H21O9), 427.1021(3.58E5; 100, C22H19O9), 409.0916(60, C22H17O8), 301.0704(10, C16H13O6), 291.0859(30, C15H15O6), 271.0597(10, C15H11O5), 247.0596(10, C13H11O5)
8.87	453.1392	C21H25O11	435.1285(50, C21H23O10), 417.1179(10, C21H21O9), 399.1072(5, C21H19O8), 315.0861(5, C17H15O6), 301.0916(15, C13H17O8), 291.0861(6.51E5; 100, C15H15O6), 273.0754(20, C15H13O5)
8.97	433.1126		
9.1	397.1133	C18H21O10	379.1022(3, C18H19O9), 235.0596(1.74E6; 100, C12H11O5), 217.0489(30, C12H9O4)
9.32	291.0877 (4.87E7)	C15H15O6	273.0756(25, C15H13O5), 165.0540(50, C9H9O3), 151.0382(25,), 139.0382(3.68E6; 100), 123.0434(90)
9.77	1019.2187		1001.2122(5), 867.1755(20), 731.1598(2.55E5; 100), 697.1544(20), 619.1075(10), 579.1126(30), 559.1227(55), 541.1122(10), 441.0813(15), 411.1074(30)
9.8	579.1493	C30H27O12	561.1394(20, C30H25O11), 543.1287(10, C30H23O10), 453.1179(5, C24H21O9), 427.1023(3.53E5; 100, C22H19O9), 409.0918(70, C22H17O8), 301.0704(15, C16H13O6), 291.0861(70, C15H15O6), 271.0598(5, C15H11O5), 247.0596(15, C13H11O5)
9.9	433.1128	C21H21O10	415.1024(60, C21H10O9), 397.0919(10, C21H17O8), 379.0812(5, C21H15O7), 271.0598(7.18E5; 100, C15H11O5)
10.12	309.0977	C15H17O7	291.0861(15, C15H15O6), 165.0539(20, C9H9O3), 147.0434(8.49E5; 100, C9H7O2))
10.15	1019.2196		1001.2126(3), 893.1910(1.56E5; 100), 867.1754(20), 729.1439(50), 697.1545(20), 603.1121(20), 559.1227(80), 541.1121(10), 419.0758(10), 407.0761(25)
10.32	397.1492	C19H25O9	235.0963(4.26E6; 100, C13H15O4)
10.35	395.1341	C19H23O9	233.0807(4.74E6; 100, C13H13O4)
10.54	291.0876	C15H15O6	273.0757(25, C15H13O5), 165.0540(50, C9H9O3), 151.0383(25,), 139.0383(3.68E6; 100), 123.0435(90)

表1 ダイオウスペクトルリスト(Pos_2)

10.57	439.1603	C21H27O10	421.1497(4.71E6; 100, C21H25O9), 277.1068(5, C15H17O5), 259.0961(15, C15H15O4)
	731.1591	C37H31O16	579.1140(40, C29H23O13), 441.0816(20, C22H17O10), 411.1075(3.89E5; 100, C22H19O8), 331.0449(5, C16H11O8), 303.0499(10, C15H11O7), 291.0862(10, C15H15O6), 271.0599(40, C15H11O5), 259.0598(10, C14H11O5)
10.65	374.124	C19H20O7N	356.1128(50, C19H18O6N), 246.0755(15, C13H12O4N), 234.0755(30, C12H12O4N), 222.0755(8.50E5; 100, C11H12O4N), 205.0488(25, C11H9O4)
10.69	1019.217		1001.2108(5), 893.1912(1.87E5; 100), 867.1757(15), 731.1597(70), 697.1544(10), 579.1124(10), 559.1227(25), 441.0814(15), 411.10731(15)
10.76	463.123	C22H23O11	445.1135(1.05E6; 100, C22H21O10), 301.0706(10, C16H13O6), 283.0600(30, C16H11O5)
10.85	344.1715	C16H26O7N	344(30), 291.1226(5, C16H19O5), 273.1118(10, C16H17O4), 255.1012(10, C16H15O3), 231.1012(20, C14H15O3), 213.0904(5, C14H13O2), 185.1954(5, C13H13O), 180.0860(15, C6H14O5N), 165.0904(50, C10H13O2), 107.0488(1.33E6; 100, C7H7O)
	191.0357 (2+)		279.0313(50,
10.88	441.0836	C11H17O13N6	381.0635(2.56E6; 100, C9H13O11N6), 331.0450(10,), 271.0601(20,), 153.0176(5,)
	517.1711 (2+)		707.1993(40,), 543.1154(10,), 435.1297(10,), 381.0634(30,), 354.1039(8.59E5; 100,), 272.0617(5,)
11.01	1171.2245		
11.17	402.1663	C20H24O6N3	385.1393(5, C20H21O6N2), 250.1183(3.11E5; 100, C12H16O3N3)
11.2	731.1591	C37H31O16	713.1520(8, C37H29O15), 605.1298(20, C31H25O13), 579.1139(90, C29H23O13), 563.1188(25, C29H23O12), 543.1290(10, C30H23O10), 455.0972(15, C23H19O10), 443.0972(40, C22H19O10), 427.1024(2.70E5; 100, C22H19O9), 409.0919(95, C22H17O8), 301.0705(40, C16H13O6), 289.0705(60, C15H13O6), 271.0599(40, C15H11O5), 259.0598(15, C14H11O5), 247.0598(40, C13H11O5)
11.23	391.1398	C20H23O8	373.1283(5, C20H21O7), 355.1177(10, C20H19O6), 229.0857(2.45E6; 100, C14H13O3)
11.33	1171.2242		1153.2209(5,), 1045.2013(40,), 1019.1865(15,), 1001.2117(15,), 883.1705(1.30E5; 100, C44H35O20), 849.1652(10, C44H33O18), 729.1440(40, C37H29O16), 711.1332(30, C37H27O15), 619.1077(35, C31H23O14), 563.1177(40, C29H23O12), 559.1228(25, C30H23O11), 541.1122(20, C30H21O10), 441.0813(35, C22H17O10)
11.45	373.1134	C16H21O10	355.1024(8.27E5; 100, C16H19O9), 337.0917(10, C16H17O8), 197.0802(60, C10H13O4), 179.0696(10H11O3)
11.51	561.1376	C30H25O11	
11.64	346.1866 329+NH3	C16H28O7N	329.1596(6.79E5; 100, C16H25O7), 293.1383(45, C16H21O5), 275.1276(80, C16H19O4), 257.1169(40, C16H17O3), 239.1061(15, C16H15O2), 233.1168(50, C14H17O3), 215.1061(35, C14H15O2), 197.0955(10, C14H13O), 167.1060(5, C10H15O2), 149.0955(30, C10H13O), 107.0489(5, C7H7O9)
11.77	1171.229		1153.2220(5,), 1045.2014(95,), 1019.1857(50,), 1001.2108(30,), 883.1702(80,), 851.1802(25,), 729.1438(60,), 711.1334(9.66E4; 100,), 563.1176(50,), 559.1226(45,), 541.1122(50,), 441.0814(50,), 409.0917(20,)
11.81	539.096		270.0521(1.61E6; 100)
11.9	285.04	C15H9O6	285(10), 267.0286(30, C15H7O5), 241.0494(1.40E6; 100, C14H9O4)
11.93	325.1135	C12H21O10	289.0916(45, C12H17O8), 271.0809(80, C12H15O7), 253.0704(10, C12H13O6), 241.0703(10, C11H13O6), 163.0594(50, C6H11O5), 145.0489(1.34E5; 100, C6H9O4), 127.0383(55, C6H7O3), 109.0279(8, C6H5O2), 97.0280(5, C5H5O2)
12	883.1693	C44H35O20	713.1489(10, C37H29O15), 579.1122(15, C29H23O13), 563.1177(9.98E5; 100, C29H23O12), 441.0813(40, C22H17O10), 409.0916(45, C22H17O8), 393.0968(30, C22H17O7), 331.0449(15, C16H11O8), 271.0602(25, C15H11O5)

表1 ダイオウスペクトルリスト(Pos_3)

12.1	561.1377	C30H25O11	543.1287(50, C30H23O10), 501.0144(40,), 409.0918(40, C22H17O8), 291.0862(2.61E5; 100, C15H15O6), 271.0600(45, C15H11O5)
12.19	505.1332	C24H25O12	191.0696(8.18E5; 100, C11H11O3)
12.22	883.1693	C44H35O20	757.1388(8, C38H29O17), 713.1490(10, C37H29O15), 579.1124(15, C29H23O13), 563.1177(8.92E5; 100, C29H23O12), 441.0812(25, C22H17O10), 409.0917(45, C22H17O8), 393.0969(30, C22H17O7), 331.0450(5, C16H11O8), 271.0602(25, C15H11O5)
12.29	460.0725(2+)		
	271.0607	C15H11O5	271(10), 253.0500(4.58E6; 100, C15H9O4), 241.0497(15, C14H9O4), 225.0546(10, C14H9O3)
12.42	463.1235	C22H23O11	301.0708(3.03E6; 100, C16H13O6)
12.51	443.0977	C22H19O10	317.0653(3, C16H13O7), 291.0860(5, C15H15O6), 273.0756(1.66E6; 100, C15H13O5), 151.0383(15, C8H7O3), 123.0435(10, C7H7O2)
12.67	505.1331		
12.7	479.1547	C23H27O11	461.1455(20, C23H25O10), 315.0713(2.44E6; 100, C13H15O9), 297.0604(10, C13H13O8), 273.0603(8, C11H13O8), 255.0497(30, C11H11O7), 237.0389(5, C11H9O6), 213.0388(8, C9H9O6), 195.0282(20, C9H7O5), 171.0282(10, C7H7O5), 153.0176(15, C7H5O4)
12.83	539.0959		270.0520(1.71E5; 100)
12.86	461.107	C22H21O11	
12.89	543.1493	C27H27O12	525.1392(45, C27H25O11), 507.1285(15, C27H23O10), 489.1179(10, C27H21O9), 465.1181(5, C25H21O9), 373.1281(8, C20H21O7), 355.1176(8, C20H19O6), 337.1070(20, C20H17O5), 315.0711(7.05E5; 100, C13H15O9), 297.0604(30, C13H13O8), 285.0604(45, C12H13O8), 271.0963(40, C16H15O4), 253.0858(C16H13O3), 241.0856(10, C15H13O3), 195.0283(8, C9H7O5), 171.0282(10, C7H7O5)
12.95	883.1668	C44H35O20	757.1391(8, C38H29O17), 713.1495(5, C37H29O15), 619.1071(5, C31H23O14), 563.1176(30, C29H23O12), 441.0814(2.18E5; 100, C22H17O10), 421.0917(45, C23H17O8), 331.0451(40, C16H11O8), 271.0604(40, C15H11O5)
13.05	419.1338	C21H23O9	419(20), 401.1233(3, C21H21O8), 257.0808(5.07E6; 100, C15H13O4)
13.21	479.1543	C23H27O11	496.1812(M+NH4) → 315.0713(2.60E6; 100, C13H15O9), 297.0604(3, C13H13O8), 171.0281(5, C7H7O5), 153.0176(5, C7H5O4)
13.34	543.149	C27H27O12	525.1390(35, C27H25O11), 507.1286(8, C27H23O10), 489.1181(10, C27H21O9), 477.1180(45, C26H21O9), 373.1281(60, C20H21O7), 355.1176(50, C20H19O6), 337.1070(20, C20H17O5), 315.0710(40, C13H15O9), 295.0963(30, C18H15O4), 285.0603(30, C12H13O8), 271.0961(10, C16H15O4), 241.0854(10, C15H13O3), 229.0854(3.65E5, 100, C14H13O3), 171.0281(5, C7H7O5)
13.46	275.0922	C15H15O5	149.0589(20, C9H9O2), 139.0382(6.05E6; 100, C7H7O3)
	584.1891		
13.73	584.1901		460.1390(10), 314.1385(4.05E5; 100)
13.86	435.1283	C21H23O10	273.0756(1.12E6; 100, C15H13O5)
13.92	461.1074	C22H21O11	
13.99	883.1695	C44H35O20	757.1389(30, C38H29O17), 713.1490(70, C37H29O15), 619.1075(5, C31H23O14), 591.1125(C30H23O13), 587.1176(50, C31H23O12), 579.1125(20, C29H23O13), 563.1176(20, C29H23O12), 543.1277(15, C30H23O10), 441.0813(1.69E5; 100, C22H17O10), 421.0916(20, C23H17O8), 409.0917(15, C22H17O8), 393.0968(10, C22H17O7), 331.0450(30, C16H11O8), 271.0602(55, C15H11O5)
14.22	465.1021	C21H21O12	303.0498(8.18E5; 100, C15H11O7)

表1 ダイオウスペクトルリスト(Pos_4)

14.31	543.1484	C27H27O12	
	271.0607	C15H11O5	229.0493(9.83E5; 100, C13H9O4), 201.0541(15, C12H9O3)
	460.0723(2+)		
14.41	275.092	C15H15O5	217.0490(40, C12H9O4), 169.0489(90, C8H9O4), 149.0590(20, C9H9O2), 127.0383(30, C6H7O3), 107.0488(3.82E5; 100, C7H7O)
14.44	395.1339	C19H23O9	377.1235(60, C19H21O8), 359.1129(15, C19H19O7), 341.1022(10, C19H17O6), 299.0915(8, C17H15O5), 275.0913(20, C15H15O5), 233.0807(2.02E6; 100, C13H13O4), 215.0699(5, C13H11O3)
14.64	515.1539	C26H27O11	303.0861(3.80E5; 100, C16H15O6), 285.0754(10, C16H13O5), 259.0960(8, C15H15O4), 177.0539(70, C10H9O3)
14.73	509.1222		240.0778(8.41E5; 100,)
14.8	475.123	C23H23O11	457.1132(9.52E5; 100,
15.03	284.1287		147.0433(9.15E5; 100,)
15.29	539.1328	C31H23O9	270.0884(4.77E5; 100, C16H14O4)
15.35	314.1396	C18H20O4N	314(15), 177.0542(2.67E6, 100, C10H9O3), 145.0278(15, C9H5O2)
15.71	461.1074	C22H21O11	443.0971(2.05E5; 100, C22H19O10), 291.0861(10, C15H15O6), 237.0390(5, C11H9O6), 147.0434(70, C9H7O2)
15.84	515.153	C26H27O11	
	409.1494	C20H25O9	373.1284(10, C20H21O7), 355.1178(8, C20H19O6), 313.1070(3, C18H17O5), 289.1070(10, C16H17O5), 247.0963(7.76E5; 100, C14H15O4)
15.91	473.1802	C25H29O9	455.1700(20, C25H27O8), 309.0967(6.79E5; 100, C15H17O7), 291.0860(5, C15H15O6), 249.0753(20, C13H13O5), 165.0539(30, C9H9O3), 147.0434(85, C9H7O2)
	309.0974	C15H17O7	291.0862(30, C15H15O6), 165.0539(5, C9H9O3), 147.0434(8.49E5; 100, C9H7O2))
16.11	461.1072	C22H21O11	
16.17	445.1127	C22H21O10	427.1023(1.36E5; 100, C22H19O9), 409.0918(5, C22H17O8), 297.0603(50, C13H13O8), 275.0911(35, C15H15O5), 257.0804(35, C15H13O4), 237.0389(20, C11H9O6), 153.0175(60, C7H5O4), 131.0485(80, C9H7O)
16.2	255.0658		
	850.2505		
16.26	409.1496	C20H25O9	373.1284(3, C20H21O7), 355.1178(3, C20H19O6), 247.0965(4.14E6; 100, C14H15O4), 229.0855(5, C14H13O3)
	391.139	C20H23O8	373.1288(70, C20H21O7), 355.1181(80, C20H19O6), 343.1181(20, C19H19O6), 325.1073(20, C19H17O5), 313.107570(70, C18H17O5), 271.0967(1.47E6; 100, C16H15O4), 259.0965(20, C15H15O4), 149.0228(5, C8H5O3)
16.39	271.0608	C15H11O5	271(50), 253.0495(80, C15H9O4), 241.0493(C14H9O4), 229.0494(1.60E6; 100, C13H9O4), 225.0545(15, C14H9O3), 201.0543(15, C12H9O3)
	919.1346 460.0721(2+)		757.0847(2.11E5; 100,), 487.0319(90,), 443.0972(15, C22H19O10), 271.0602(65, C15H11O5)
16.45	461.1068	C22H21O11	
16.58	255.0658	C15H11O4	
	256.5360 (2+)		350.0110(10,), 255.0650(55, C15H11O4), 237.0542(15, C15H9O3), 227.0699(4.67E5; 100, C14H11O3), 209.0592(25, C14H9O2), 199.0749(20, C13H11O2), 181.0642(10, C13H9O), 135.0434(10, C8H7O2), 121.0277(5, C7H5O2)
	850.2532		325.1131(10,), 255.0651(3.05E5; 100, C15H11O4)

表1 ダイオウスペクトルリスト(Pos_5)

16.6	255.0658	C15H11O4	
	256.5361(2+)		350.0113(3.52E5; 100,), 255.0650(35, C15H11O4), 236.0218(10,), 227.0698(65, C14H11O3), 214.9871(30,), 209.0591(15, C14H9O2), 199.0748(15, C13H11O2), 181.0642(8, C13H9O), 145.0488(20, C6H9O4), 127.0383(5, C6H7O3)
16.62	519.1125	C24H23O13	501.1028(30, C24H21O12), 483.0922(15, C24H19O11), 379.0812(10, C21H15O7), 337.0706(20, C19H13O6), 313.0706(30, C17H31O6), 295.0599(5, C17H11O5), 271.0599(6.34E5; 100, C15H11O5)
16.71	475.2115		377.1278(85,), 311.1501(3.14E6; 100,)
16.78	419.1338	C21H23O9	
16.87	230.1758	C12H24O3N	212.1646(4.84E6; 100, C12H22O2N)
	212.165	C12H22O2N	212(20), 194.1542(6.78E6; 100, C12H20ON), 166.1590(30, C11H20N), 149.1322(5, C11H17)
16.94	495.1489	C23H27O12	477.1392(1.25E6; 100, C23H25O11), 459.1286(20, C23H23O10), 355.1176(10, C20H19O6), 313.1069(15, C18H17O5)), 289.1068(20, C16H17O5), 271.0961(15, C16H15O4), 247.0961(40, C14H15O4), 229.0853(10, C14H13O3)
17.0	461.1079	C22H21O11	443.0977(2.21E6; 100, C22H19O10), 291.0862(10, C15H15O6), 237.0388(5, C11H9O6), 147.0434(70, C9H7O2)
	340.0596 (2+)		533.0746(30,), 509.0895(10,), 363.0527(55,), 331.0537(2+; 25,), 322.0485(2+; 10,), 255.0480(2+; 7.06E5; 100,), 147.0434(70,)
	642.2164	C32H36O13N	461.1080(2.16E6; 100, C22H21O11)
17.16	461.1078	C22H21O11	443.0973(15, C22H19O10), 297.0603((20, C13H13O8), 291.0861(10, C15H15O6), 147.0434(9.30E5; 100, C9H7O2)
	340.0595 (2+)		533.0746(4.02E5; 100,), 255.0479(5,), 147.0434(65,)
	642.2164	C32H36O13N	625 → 607.1818(25, C32H31O12), 589.1711(10, C32H29O11), 461.1079(2.87E5; 100, C22H21O11), 455.1701(10, C25H27O8), 419.0974(10, C20H19O10), 401.0866(10, C20H17O9), 273.0755(15, C15H13O5), 255.0495(8, C11H11O7)
17.52	461.1078	C22H21O11	443.0975(15, C22H19O10), 297.0603((10, C13H13O8), 291.0862(40, C15H15O6), 147.0434(9.30E5; 100, C9H7O2)
	340.0596 (2+)		533.0746(9.33E5; 100,), 147.0434(65,)
	642.2164	C32H36O13N	625 → 607.1816(25, C32H31O12), 589.1707(5, C32H29O11), 461.1077(3.61E5; 100, C22H21O11), 455.1700(15, C25H27O8), 419.0972(5, C20H19O10), 291.0861(10, C15H15O6), 255.0495(3, C11H11O7), 165.0539(30, C9H9O3)
17.65	285.0766	C16H13O5	285(5.09E6; 100), 267.0654(10, C16H11O4), 257.0809(10, C15H13O4), 253.0496(10, C15H9O4), 239.0703(8, C15H11O3), 211.0752(8, C14H11O2)
17.81	255.1598	C14H23O4	237.1482(1.54E6; 100, C14H21O3), 219.1375(40, C14H19O2), 201.1268(10, C14H17O), 183.1161(5, C14H15), 159.1161(3, C12H15), 137.1318(3, C10H17), 121.1006(3, C9H13)
17.91	445.1126	C22H21O10	427.1024(2.72E5; 100, C22H19O9), 315.0708(5, C13H15O9), 297.0603(40, C13H13O8), 275.0911(35, C15H15O5), 261.0390(5, C13H9O6), 237.0389(5, C11H9O6), 153.0175(25, C7H5O4), 131.0485(30, C9H7O)
18.27	285.0765	C16H13O5	285(1.04E5; 100), 270.0520(60, C15H10O5), 267.0649(65, C16H11O4), 257.0805(60, C15H13O4), 253.0493(60, C15H9O4), 242.0570(65, C14H10O4), 239.0699(65, C15H11O3), 225.0541(20, C14H9O3), 211.0749(90, C14H11O2), 151.0383(15, C8H7O3)
18.3	244.1914	C13H26O3N	226.1806(7.32E6; 100, C13H24O2N)
18.6	348.2749	C18H38O5N	313.2374(15, C18H33O4), 295.2267(40, C18H31O3), 277.2160(8, C18H29O2), 213.1480(65, C12H21O3), 195.1374(3.70E5; 100, C12H19O2), 173.1166(15, C9H17O3), 30, C9H15O2)
18.7	298.1445	C18H20O3N	177.0540(1.69E6; 100, C10H9O3), 145.0277(15, C9H5O2)

表1 ダイオウスペクトルリスト(Pos_6)

	451.1597	C22H27O10	433.1493(3.32E5; 100, C22H25O9), 415.1388(20, C22H23O8), 397.1283(10, C22H21O7), 355.1176(15, C20H19O6), 337.1070(10, C20H17O5), 313.1068(10, C18H17O5), 289.1068(20, C16H17O5), 271.0961(10, C16H15O4), 247.0961(85, C14H15O4), 229.0854(8, C14H13O3)
19.07	457.1855	C25H29O8	439.1753(25, C25H27O7), 421.1645(3, C25H25O6), 403.1540(5, C25H23O5), 293.1019(1.21E6; 100, C15H17O6), 273.1118(10, C16H17O4), 255.1012(5, C16H15O3), 233.0804(50, C13H13O4), 191.0696(3, C11H11O3), 149.0590(15, C9H9O2), 131.0485(C9H7O)
19.15	213.1488	C12H21O3	195.1374(30, C12H19O2), 177.1268(40, C12H17O), 167.1425(5.40E5; 100, C11H19O), 159.1162(45, C12H15), 149.1319(95, C11H17), 135.1161(10, C10H15)
19.16	231.1594	C12H23O4	213.1480(1.47E6; 100, C12H21O3)
19.2	256.1914	C14H26O3N	238.1801(2.03E6; 100, C14H24O2N)
19.26	445.1125	C22H21O10	427.1024(1.62E5; 100, C22H19O9), 297.0603(60, C13H13O8), 275.0911(65, C15H15O5), 261.0391(5, C13H9O6), 237.0389(5, C11H9O6), 153.0176(40, C7H5O4), 131.0485(45, C9H7O)
19.46	331.1908	C20H27O4	313.1797(5, C20H25O3), 285.1847(10, C19H25O2), 243.1738(3, C17H23O), 227.1424(C16H19O), 203.1061(6.92E5; 100, C13H15O2)
19.73	258.2068	C14H28O3N	240.1956(2.01E6; 100, C14H26O2N)
	240.1962	C14H26O2N	240(20), 222.1849(1.86E6; 100, C14H24ON), 204.1740(5, C14H22N), 194.1898(20, C13H24N)
19.9	609.1951 626.2220(609+NH 3)	C32H33O12	626 → 609.1975(5, C32H33O12), 445.1133(3.02E6; 100, C22H21O10), 427.1026(5, C22H19O9), 297.0603(10, C13H13O8), 257.0804(C15H13O4)
19.99	445.1131	C22H21O10	427.1024(2.71E5; 100, C22H19O9), 297.0603(95, C13H13O8), 275.0911(60, C15H15O5), 261.0391(10, C13H9O6), 237.0389(10, C11H9O6), 171.0281(10, C7H7O5), 153.0176(45, C7H5O4), 131.0485(60, C9H7O)
	1053.2935		
20.02	332.0620 (2+)		533.0745(20,), 493.0946(15,), 363.0526(20,), 323.0563(2+, 40,), 314.0510(2+, 8,), 247.0506(2+, 8.48E5; 100,), 153.0175(10,), 131.0485(25,)
20.62	609.1957 626.2221(609+NH 3)	C32H33O12	626 → 609.1973(25, C32H33O12), 445.1129(5.15E5; 100, C22H21O10), 275.0911(10, C15H15O5)
			609 → 591.1868(95, C32H31O11), 573.1760(10, C32H29O10), 461.1443(80, C23H25O10), 445.1131(4.86E5; 100, C22H21O10), 439.1755(30, C25H27O7), 425.1232(8, C23H21O8), 403.1540(8, C25H23O5), 385.0918(10, C20H17O8), 273.1120(15, C16H17O4), 255.0498(15, C11H11O7), 233.0805(10, C13H13O4)
	445.113	C22H21O10	427.1022(80, C22H19O9), 297.0602(85, C13H13O8), 275.0910(4.66E5; 100, C15H15O5), 257.0804(15, C15H13O4), 237.0387(5, C11H9O6), 191.0694(3, C11H11O3), 153.0175(65, C7H5O4), 131.0484(80, C9H7O)
	332.0622 (2+)		533.0744(45,), 511.1053(6.07E5; 100,), 153.0175(70,), 131.0485(20,)
21.18	272.2226	C15H30O3N	254.2114(1.55E6; 100, C15H28O2N)

表2 ダイオウスペクトルリスト(Neg_1)

保持時間 (min)	m/z	推定組成	プロダクトイオン
2.33	201.0251		201(2.74E4; 100,), 157.0352(95,)
2.62	401.1294	C14H25O13	341.1085(2.17E6; 100, C12H21O11)
2.71	470.1509 453+NH3	C17H28O14N	341.1082(2.40E5; 100, C12H21O11)
2.99	439.0751		421.0739(30,), 341.1079(1.79E4; 100,), 277.0323(70,), 259.0216(80,)
3.88	257.0774		238.0827(5,), 128.0351(1.55E5; 100,)
4.27	493.1186	C19H25O15	331.0662(7.66E5; 100, C13H15O10)
4.31	331.0663	C13H15O10	313.0559(20, C13H13O9), 271.0456(1.68E5; 100, C11H11O8), 241.0347(15, C10H9O7), 223.0243(15, C10H7O6), 211.0244(40, C9H7O6), 193.0140(80, C9H5O5), 169.0141(70, C7H5O5), 151.0034(10,)
4.48	339.0352	C14H11O10	169.0137(5.24E5; 100, C7H5O5)
	169.014	C7H5O5	169(4.31E5; 100), 125.0244(50,
4.61	493.1193	C19H25O15	433.0978(3, C17H21O13), 331.0663(15, C13H15O10), 313.0558(3.30E5; 100, C13H13O9), 271.0453(40, C11H11O8), 241.0346(3, C10H9O7), 211.0241(2, C9H7O6), 169.0138(C7H5O5)
4.87	287.04	C11H11O9	269.0294(5, C11H9O8), 169.0140(6.27E4; 100, C7H5O5), 135.0296(80,)
5	331.0665	C13H15O10	313.0558(10, C13H13O9), 271.0455(1.37E5; 100, C11H11O8), 241.0349(60, C10H9O7), 223.0243(15, C10H7O6), 169.0140(60, C7H5O5)
5.18	323.1343	C13H23O9	241.0347(3.20E4; 100, C10H9O7), 179.0556(20, C6H11O6)
5.31	669.1656	C29H33O18	609.1448(1.70E5; 100, C27H29O16), 447.0924(40, C21H19O11)
5.44	483.0767	C20H19O14	439.0872(5, C19H19O12), 331.0664(1.37E5; 100, C13H15O10), 313.0557(5, C13H13O9), 169.0139(10, C7H5O5)
5.57	345.082	C14H17O10	183.0297(5.76E4; 100, C8H7O5)
5.79	483.077	C20H19O14	465.0663(20, C20H17O13), 439.0871(40, C19H19O12), 331.0663(70, C13H15O10), 313.0558(2.83E4; 100, C13H13O9), 271.0453(70, C11H11O8), 211.0242(30, C9H7O6), 193.0137(50, C9H5O5)169.0139(10, C7H5O5)
5.92	451.1235	C21H23O11	299.0767(10, C13H15O8), 289.0712(4.02E5; 100, C15H13O6)
5.96	359.1338	C16H23O9	299.1131(1.79E5; 100, C14H19O7), 161.0452(10, C6H9O5), 137.0606(10,)
6.13	384.129	C17H22O9N	340.1394(20, C16H22O7N), 307.0816(10, C15H15O7), 178.0871(2.04E4; 100, C10H12O2N)
8.51	451.1236	C21H23O11	289.0712(1.54E5; 100, C15H13O6), 245.0812(5, C14H13O4)
8.56	203.0821	C11H11O2N2	186.0555(20, C11H8O2N), 159.0925(2.80E4; 100, C10H11N2), 142.0659(8, C10H8N), 116.0507(5,)
8.77	483.0769	C20H19O14	465.0661(10, C20H17O13), 439.0869(50, C19H19O12), 423.0558(80, C18H15O12), 405.0453(5, C18H13O11), 331.0660(30, C13H15O10), 313.0556(3.98E4; 100, C13H13O9), 295.0449(15, C13H11O8), 271.0451(90, C11H11O8), 241.0345(20, C10H9O7), 211.0240(30, C9H7O6), 193.0136(35, C9H5O5), 169.0139(30, C7H5O5)

表2 ダイオウスペクトルリスト(Neg_2)

9.08	865.1961	C45H37O18	
9.3	451.1239	C21H23O11	289.0712(1.54E5; 100, C15H13O6)
	325.0921	C15H17O8	307.0818(1.37E5; 100, C15H15O7), 265.0711(5, C13H13O6), 245.0813(5, C14H13O4), 217.0500(15, C12H9O4), 187.0397(20, C11H7O3)
9.34	295.0818	C14H15O7	277.0714(50, C14H13O6), 251.0920(10, C13H15O5), 233.0814(4.06E5; 100, C13H13O4)
9.38	483.0774	C20H19O14	465.0661(3, C20H17O13), 423.0561(2.83E5; 100, C18H15O12), 405.0453(5, C18H13O11), 331.0662(10, C13H15O10), 313.0558(15, C13H13O9), 295.0450(5, C13H11O8), 271.0453(30, C11H11O8), 241.0346(3, C10H9O7), 211.0242(10, C9H7O6), 193.0137(10, C9H5O5), 169.0138(5, C7H5O5)
9.47	865.1968	C45H37O18	
9.51	577.1343	C30H25O12	577(40), 559.1245(10, C30H23O11), 451.1031(35, C24H19O9), 425.0874(7.26E5; 100, C22H17O9), 407.0771(85, C22H15O8), 299.0559(10, C16H11O6), 289.0715(30, C15H13O6)
9.56	483.0768	C20H19O14	465.0663(5, C20H17O13), 439.0872(6.80E5; 100, C19H19O12), 423.0562(5, C18H15O12), 331.0663(5, C13H15O10), 313.0558(10, C13H13O9), 287.0764(3, C12H15O8), 271.0453(25, C11H11O8), 211.0243(10, C9H7O6), 193.0138(10, C9H5O5)
9.68	359.134	C16H23O9	
	325.0923	C15H17O8	
9.75	577.1342	C30H25O12	577(60), 559.1242(10, C30H23O11), 451.1031(35, C24H19O9), 425.0874(7.37E5; 100, C22H17O9), 407.0769(70, C22H15O8), 299.0558(10, C16H11O6), 289.0714(25, C15H13O6)
9.77	241.0349(2-)	C20H18O14	313.0561(75, C13H13O9), 271.0454(50, C11H11O8), 232.0296(2-, 35, C20H16O13), 211.0245(60, C9H7O6), 169.0141(6.65E4; 100, C7H5O5)
	321.0608	C15H13O8	303.0506(10, C15H11O7), 277.0714(5.08E5; 100, C14H13O6), 259.0609(10, C14H11O5), 233.0817(70, C13H13O4), 215.0711(5, C13H11O3)
9.81	483.0772	C20H19O14	465.0663(5, C20H17O13), 439.0875(2.04E5; 100, C19H19O12), 423.0559(10, C18H15O12), 331.0662(15, C13H15O10), 313.0557(20, C13H13O9), 271.0453(50, C11H11O8), 241.0346(3, C10H9O7), 211.0241(8, C9H7O6), 193.0137(5, C9H5O5), 169.0138(3, C7H5O5)
	451.124	C21H23O11	289.0711(1.44E6; 100, C15H13O6), 245.0815(5, C14H13O4)
9.86	325.0921	C15H17O8	
	653.1711 593+AcOH	C29H33O17	593.1501(2.20E5; 100, C27H29O15), 431.0975(60, C21H19O10)
9.9	669.1662	C29H33O18	
10.03	295.0816	C14H15O7	277.0714(50, C14H13O6), 251.0921(10, C13H15O5), 233.0814(6.01E5; 100, C13H13O4)
10.12	483.0772	C20H19O14	439.0873(5, C19H19O12), 331.0663(8, C13H15O10), 313.0557(7.18E5; 100, C13H13O9), 169.0139(10, C7H5O5)
10.16	865.1969	C45H37O18	847.1854(15,), 739.1647(50, C39H31O15), 713.1493(40, C37H29O15), 695.1392(1.42E5; 100, C37H27O14), 587.1178(20, C31H23O12), 577.1337(70, C30H25O12), 543.0917(15, C29H19O11), 451.1022(15, C24H19O9), 425.0865(17, C22H17O9), 407.0761(20, C22H15O8), 287.0553(17, C15H11O6)

表2 ダイオウスペクトルリスト(Neg_3)

10.2	325.0923	C15H17O8	
	321.0611	C15H13O8	303.0505(15, C15H11O7), 277.0711(6.21E5; 100, C14H13O6), 259.0606(10, C14H11O5), 233.0817(80, C13H13O4), 215.0708(5, C13H11O3)
10.26	289.0713 (2.50E7)	C15H13O6	289(30), 245.0815(5.38E6; 100, C14H13O4), 205.0503(40, C11H9O4), 179.0348(15, C9H7O4)
10.52	325.0923	C15H17O8	
10.58	431.1549	C19H27O11	
10.6	865.1964	C45H37O18	
10.65	577.1345	C30H25O12	559.1235(10, C30H23O11), 451.1028(30, C24H19O9), 425.0870(4.16E5; 100, C22H17O9), 407.0766(50, C22H15O8), 299.0555(5, C16H11O6), 289.0712(20, C15H13O6)
	508.1001 (2-)	C52H40O22	891.1756(30,), 847.1851(5,), 739.1650(7,), 727.1289(60, C37H27O16), 713.1449(30,), 695.1392(30,), 677.1282(5,), 603.1130(10,), 575.1180(20,), 432.0764(2+; 85, C44H32O19), 423.0712(2+; 1.20E5; 100, C44H30O18), 303.0503(65,), 289.0711(60,)
	653.1714 593+AcOH	C29H33O17	593.1503(8.19E5; 100, C27H29O15), 431.0980(10, C21H19O10)
10.73	325.0922	C15H17O8	307.0818(15, C15H15O7), 289.0713(7, C15H13O6), 265.0713(70, C13H13O6), 235.0606(30, C12H11O5), 217.0501(10, C12H9O4), 205.0502(20, C11H9O4), 187.0397(5.46E4; 100, C11H7O3), 163.0398(90, C9H7O3), 145.0292(50, C9H5O2)
10.78	547.2024		
10.86	329.0872	C14H17O9	167.0345(3.19E5; 100, C8H7O2)
10.91	508.1001 (2-)	C52H40O22	891.1761(30, C46H35I9), 865.1607(5, C44H33O19), 739.1654(10,), 727.1293(60, C37H27O16), 713.1502(25,), 695.1393(30,), 677.1287(5,), 603.1130(10,), 575.1182(20,), 432.0766(2+; 85, C44H32O19), 423.0713(2+; 1.20E5; 100, C44H30O18), 303.0504(60,), 289.0711(75,)
10.95	728.1346 (2-)		1331.2485(20,), 1287.2592(25,), 1169.2167(50,), 665.1202(2-; 25,), 652.1282(2-; 30,), 643.1075(2-; 95,), 583.0967(2-; 50,), 575.1176(45,), 439.0695(5.41E4; 100,), 289.0707(30,)
10.99	325.0922	C15H17O8	
11.08	455.1555	C21H27O11	395.1341(10, C19H23O9), 233.0813(7.46E5; 100, C13H13O4)
	635.0883	C27H23O18	465.0663(8.91E5; 100, C20H17O13)
11.12	728.1374 (2-)		
11.16	393.1187	C19H21O9	
11.25	653.1709		
	729.145	C37H29O16	729(90), 603.1136(10, C31H23O13), 577.1345(2.32E6; 100, C30H25O12), 559.1244(40, C30H23O11), 541.1138(5, C30H21O10), 451.1031(15, C24H19O9), 433.0926(10, C27H17O8), 425.0875(25, C22H17O9), 407.0770(45, C22H15O8), 289.0715(8, C15H13O6)
11.26	577.1343	C30H25O12	

表2 ダイオウスペクトルリスト(Neg_4)

11.31	289.0713	C15H13O6	289(30), 245.0815(4.22E6; 100, C14H13O4), 205.0503(40, C11H9O4), 179.0348(15, C9H7O4)
11.39	325.0924	C15H17O8	
	635.0886	C27H23O18	617.0767(5, C27H21O17), 591.0975(5, C26H23O16), 483.0771(80, C20H19O14), 465.0665(3.89E5; 100, C20H17O13), 423.0561(20, C18H15O12), 313.0559(30, C13H13O9), 271.0453(10, C11H11O8), 221.0450(10, C11H9O5)
11.55	729.1453	C37H29O16	729(60), 603.1136(10, C31H23O13), 577.1343(1.38E6; 100, C30H25O12), 559.1238(15, C30H23O11), 559.0877(35, C29H19O12), 541.1133(5, C30H21O10), 451.1028(30, C24H19O9), 441.0822(35, C22H17O10), 407.0767(70, C22H15O8), 289.0713(15, C15H13O6)
11.67	385.1501	C18H25O9	385(20), 325.1268(3.48E6; 100, C16H21O7), 163.0761(30, C10H11O2)
11.8	729.1452	C37H29O16	729(4.51E6; 100), 711.1349(10, C37H27O15), 603.1136(25, C31H23O13), 577.1342(25, C30H25O12), 559.1243(40, C30H23O11), 541.1138(5, C30H21O10), 451.1031(15, C24H19O9), 433.0925(10, C27H17O8), 425.0875(25, C22H17O9), 407.0769(45, C22H15O8), 289.0714(10, C15H13O6)
11.9	449.1447	C22H25O10	449(10), 389.1239(90, C20H21O8), 227.0711(2.71E6; 100, C14H11O3)
12.07	415.1608	C19H27O10	355.1389(3.68E5; 100, C17H23O8), 289.0710(15, C15H13O6), 193.0865(30, C11H13O3), 161.0452(15, C6H9O5)
12.15	861.1872 430.0900(2-)	C42H37O20	430(2-) → 592.1427(5, C27H28O15), 431.0953(10,), 389.0871(9.79E5; 100, C19H17O9), 268.0373(20, C15H8O5), 227.0345(25, C13H7O4)
12.23	1069.2183 584.1061(2-)	C59H41O20	584(2-) → 1043.1864(15,), 999.1964(20,), 891.1752(10,), 879.1394(35,), 865.1599(20,), 847.1498(50,), 727.1286(20,), 603.1127(10,), 521.0892(10,), 508.0999(2-, 1.12E5; 100,), 499.0766(30,), 439.0659(10,), 303.0503(60,), 289.0710(30,)
	847.2077	C42H39O19	
12.39	445.0771	C21H17O11	445(20), 325.0350(15, C17H9O7), 307.0245(10, C17H7O6), 297.0401(8, C16H9O6), 283.0245(4.99E6; 100, C15H7O6), 269.0452(25, C15H9O5), 239.0348(10, C14H7O4)
12.47	881.1565 440.0748(2-)	C44H33O20	
12.6	728.1376 (2-)		
12.68	881.1560 440.0742(2-)	C44H33O20	440(2-) → 755.1241(3, C38H27O17), 711.1346(5, C37H27O15), 603.1135(10, C31H23O13), 577.0981(30, C29H21O13), 559.0877(50, C29H19O12), 407.0768(40, C22H15O8), 364.0689(2-, 50, C37H28O16), 303.0506(6.45E5; 100, C15H11O7), 289.0714(10, C15H13O6)
	431.0979	C21H19O10	413.0871(3, C21H17O9), 341.0659(3, C18H13O7), 311.0555(15, C17H11O6), 283.0606(10, C16H11O5), 269.0449(6.25E5; 100, C15H9O5)
12.8	461.1086	C22H21O11	417.1185(1.42E6; 100, C21H21O9), 256.0690(5,)
12.88	729.1454	C37H29O16	729(7.60E5; 100), 711.1355(5, C37H27O15), 603.1142(25, C31H23O13), 577.1348(35, C30H25O12), 559.1245(15, C30H23O11), 541.1138(3, C30H21O10), 451.1033(20, C24H19O9), 441.0827(15, C22H17O10), 433.0927(5, C27H17O8), 425.0876(5, C22H17O9), 407.0771(40, C22H15O8), 289.0716(10, C15H13O6)
12.98	441.0819	C22H17O10	441(40), 397.0926(3, C21H17O8), 331.0456(20, C16H11O8), 303.0506(10, C15H11O7), 289.0712(8.07E6; 100, C15H13O6), 271.0609(15, C15H11O5), 245.0815(3, C14H13O4), 193.0140(8,), 169.0141(15, C7H5O5)

表2 ダイオウスペクトルリスト(Neg_5)

13.06	861.1881	C42H37O20	
13.1	477.1395	C23H25O11	477(95), 441.0825(10, C22H17O10), 313.0560(2.33E6; 100, C13H13O9), 169.0141(25, C7H5O5)
13.17	541.1342	C27H25O12	541(95), 313.0558(1.32E7; 100, C13H13O9), 227.0709(10, C14H11O3), 169.0141(10, C7H5O5)
13.3	881.1550 440.0746(2-)	C44H33O20	
13.5	477.1394	C23H25O11	477(90), 313.0561(8.68E6; 100, C13H13O9), 253.0352(3, C11H9O7), 169.0142(25, C7H5O5)
13.61	541.1345	C27H25O12	541(6.33E5; 100), 379.0815(3, C21H15O7), 313.0558(80, C13H13O9), 227.0709(10, C14H11O3), 169.0140(5, C7H5O5)
13.9	744.2284		431.0973(3.26E5; 100, C21H19O9), 269.0447(5, C15H9O5)
14.08	629.1141 314.0534(2-)	C29H25O16	585.1237(60, C28H25O14), 477.1028(1.17E5; 100, C22H21O12), 465.0662(10, C20H17O13), 459.0924(80, C22H19O11), 417.0817(C20H17O10), 313.0555(5, C13H13O9), 271.0451(20, C11H11O8)
14.12	881.1544 440.0743(2-)	C44H33O20	440(2-) → 755.1230(5, C38H27O17), 711.1334(3, C37H27O15), 603.1124(15, C31H23O13), 577.0972(45, C29H21O13), 559.0867(35, C29H19O12), 407.0762(30, C22H15O8), 364.0684(2-, 70, C37H28O16), 303.0502(2.75E5; 100, C15H11O7), 288.0449(2-, 5, C29H20O13)
14.29	459.0925	C22H19O11	325.0711(5, C18H13O6), 295.0608(60, C17H11O5), 267.0658(C16H11O4), 253.0501(4.19E5; 100, C15H9O4)
14.45	431.0977	C21H19O10	431(40), 269.0451(6.77E6; 100, C15H9O5)
14.49	629.1140 314.0533(2-)	C29H25O16	
	847.2074	C42H39O19	
14.54	435.1288	C21H23O10	435(15), 273.0764(1.69E6; 100, C15H13O5)
14.61	393.1187	C19H21O9	231.0658(2.83E6; 100, C13H11O4)
14.66	487.0875	C23H19O12	487(40), 325.0348(10, C17H9O7), 307.0243(5, C17H7O6), 283.0243(60, C15H7O6), 263.0345(15, C16H7O4), 239.0344(7.67E5; 100, C14H7O4)
	473.1443		
14.7	187.0971	C9H15O4	187(95), 125.0969(1.52E5; 100, C8H13O)
14.79	861.187	C42H37O20	
14.87	473.1085	C23H21O11	311.0557(10, C17H11O6), 293.0450(5, C17H9O5), 269.0450(9.21E5; 100, C15H9O5), 253.0502(3, C15H9O4), 217.0350(3, C8H9O7)
	509.1444	C27H25O11	473.1074(5, C23H21O11), 281.0658(5.72R5; 100, C13H13O7), 269.0446(5, C15H9O5), 227.0706(20, C14H11O3)
14.91	431.1545	C19H27O11	
	371.1333	C17H23O9	209.0815(6.67E5; 100, C11H13O4)
	461.108	C22H21O11	443.0974(5, C22H19O10), 401.0873(70, C20H17O9), 313.0560(2.42E5; 100, C13H13O9), 295.0453(10, C13H11O8), 253.0347(3, C11H9O7), 241.0347(3, C10H9O7), 223.0242(3, C10H7O6), 211.0242(10, C9H7O6), 193.0137(8, C9H5O5), 169.0140(15, C7H5O5)

表2 ダイオウスペクトルリスト(Neg_6)

15.0	705.1489 352.07 (2-)		352 → 607.1780(15,), 459.0909(80,), 312.0910(2-, 50,), 279.0513(25, C13H11O7), 271.0597(15, C15H11O5), 245.0477(8.74E4; 100,), 169.0134(5, C7H5O5)
15.13	861.2239		817.2300(3,), 699.1682(2.83E5; 100,), 681.1573(3,), 655.1777(3,), 537.1157(10,), 493.1262(3, C30H21O7), 389.0855(20, C19H17O9)
15.17	227.0704	C14H11O3	227(3.53E5; 100), 185.0600(50, C12H9O2), 159.0808(10, C11H11O), 143.0496(3, C10H7O)
15.2	461.1086	C22H21O11	401.0873(2.69E5; 100, C20H17O9), 313.0553(350, C13H13O9), 299.0550(15, C16H11O6), 295.0448(5, C13H11O8), 271.0450(60, C11H11O8), 211.0240(10, C9H7O6), 169.0138(15, C7H5O5)
15.3	352.0703 (2-)		
15.43	214.1441	C11H20O3N	214(10), 197.1176(2.69E5; 100, C11H17O3), 153.1280(80, C10H17O)
15.47	312.1235	C18H18O4N	312(3.15E5; 100), 297.0996(60, C17H15O4N), 270.1124(10, C16H16O3N), 253.0859(5, C16H13O3), 178.0504(40, C9H8O3N), 135.0447(10, C8H7O2)
15.6	625.1556	C31H29O14	459.0910(4.80E5; 100, C22H19O11)
	699.1347	C36H27O15	655.1417(20,), 579.0897(3,), 537.0799(2.59E5; 100, C30HH17O10), 519.0692(3,), 493.0903(8, C29H17O8), 389.0859(5, C19H17O9), 227.0340(5, C13H7O4)
15.69	461.1086	C22H21O11	443.0965(20, C22H19O10), 401.0864(9.73E4; 100, C20H17O9), 313.0555(80, C13H13O9), 295.0449(5, C13H11O8), 271.0449(10, C11H11O8), 253.0344(3, C11H9O7), 239.0705(40, C15H11O3), 211.0240(60, C9H7O6), 193.0136(45, C9H5O5), 169.0138(70, C7H5O5)
15.81	471.1657	C25H27O9	471(60), 307.0812(1.48E6; 100, C15H15O7), 247.0604(5, C13H11O5), 187.0396(5, C11H7O3), 163.0398(5, C9H7O3), 145.0293(5, C9H5O2)
15.85	613.1197		
15.94	461.108	C22H21O11	443.0963(25, C22H19O10), 401.0862(9.16E4; 100, C20H17O9), 313.0553(60, C13H13O9), 295.0445(5, C13H11O8), 253.0341(5, C11H9O7), 223.0238(5, C10H7O6), 211.0240(70, C9H7O6), 193.0135(40, C9H5O5), 169.0137(50, C7H5O5)
	699.1349	C36H27O15	
15.98	623.1764	C32H31O13	477.1379(10, C23H25O11), 459.0916(1.82E5; 100, C22H19O11), 313.0554(8, C13H13O9), 295.0449(15, C13H11O8)
16.07	461.1085	C22H21O11	
	415.1031	C21H19O9	415(10), 357.0972(3, C19H17O7), 325.0712(3, C18H13O6), 295.0606(15, C17H11O5), 277.0500(8, C17H9O4), 277.0656(10, C16H11O4), 253.0501(1.24E6; 100, C15H9O4)
16.13	407.134	C20H23O9	245.0808(9.45E5; 100, C14H13O4)
16.17	847.2097	C42H39O19	
16.21	431.0973	C21H19O10	431(40), 311.0554(15, C17H11O6), 293.0448(5, C17H9O5), 269.0447(5.64E6; 100, C15H9O5)
16.38	415.103	C21H19O9	397.0917(5, C21H17O8), 357.0969(3, C19H17O7), 325.0709(5, C18H13O6), 295.0606(15, C17H11O5), 277.0500(8, C17H9O4), 267.0656(10, C16H11O4), 253.0500(6.14E5; 100, C15H9O4)

表2 ダイオウスペクトルリスト(Neg_7)

16.51	613.1193	C29H25O15	461.1068(80, C22H21O11), 443.0966(7.42E4; 100, C22H19O10), 401.0860(50, C20H17O9), 313.0551(10, C13H13O9), 295.0445(5, C13H11O8), 271.0447(20, C11H11O8)
16.63	623.1767	C32H31O13	623(20), 459.0912(1.76E6; 100, C22H19O11), 315.0500(5, C16H11O7), 295.0450(5, C13H11O8)
	517.0989	C23H21O13	473.1075(2.69E6; 100, C23H21O11)
	228.1597	C12H22O3N	228(1.12E6; 100), 211.1334(90, C12H19O3), 167.1439(80, C11H19O)
16.67	449.1448	C22H25O10	389.1225(3, C20H21O8), 245.0810(1.08E6; 100, C14H13O4), 230.0579(5, C13H10O4)
16.76	457.1136	C23H21O10	295.0599(10, C17H11O5), 277.0494(5, C17H9O4), 267.0650(3, C16H114), 253.0494(1.04E6; 100, C15H9O4)
16.8	623.1765	C32H31O13	623(1.18E6; 100), 477.1384(30, C23H25O11), 471.1643(10, C25H27O9), 459.0917(45, C22H19O11), 313.0555(5, C13H13O9), 307.0815(10, C15H15O7)
16.84	653.187	C33H33O14	635.1728(10,), 609.1575(15,), 593.1622(10,), 501.1737(15,), 489.1015(1.04E5; 100, C23H21O12), 477.1377(15, C23H25O11), 469.1480(40, C25H25O9), 459.1273(15, C23H23O10), 443.0961(40, C22H19O10), 337.0914(5, C16H17O8), 323.0757(20, C15H15O8), 295.0446(5, C13H11O8)
16.88	445.1133	C22H21O10	427.1013(3, C22H19O9), 355.0808(5, C19H15O7), 325.0704(20, C18H13O6), 297.0757(10, C17H13O5), 283.0601(4.13E5; 100, C16H11O5)
17.01	457.1136	C23H21O10	295.0601(10, C17H11O5), 277.0495(5, C17H9O4), 267.0651(3, C16H114), 253.0495(8.13E5; 100, C15H9O4)
17.09	623.1769	C32H31O13	623(1.92E6; 100), 477.1382(10, C23H25O11), 471.1641(20, C25H27O9), 459.0914(45, C22H19O11), 313.0553(5, C13H13O9), 307.0814(10, C15H15O7), 295.0449(5, C13H11O8)
	327.1807		
17.21	445.1137	C22H21O10	427.1019(3, C22H19O9), 413.0864(3, C21H17O9), 325.0708(10, C18H13O6), 297.0759(5, C17H13O5), 283.0603(1.07E6; 100, C16H11O5)
17.3	653.186	C33H33O14	
17.34	327.2172	C18H31O5	327(60), 309.2061(15, C18H29O4), 291.1958(50, C18H27O3), 273.1851(10, C18H25O2), 247.2059(10, C17H27O), 239.1282(20, C13H19O4), 229.1439(2.56E5; 100, C12H21O4), 221.1178(25, C13H17O3), 211.1135(70, C12H19O3), 209.1178(20, C12H17O3), 203.1072(3, C13H15O2), 197.1177(3, C11H17O3), 193.1593(5, C13H21O), 183.1386(5, C11H19O2), 177.1281(3, C12H17O), 171.1024(35, C9H15O3), 165.1281(5, C11H17O)
17.43	473.1085	C23H21O11	473(15), 311.0551(10, C17H11O6), 293.0446(5, C17H9O5), 269.0446(8.62E5; 100, C15H9O5)
17.47	607.1816	C32H31O12	459.1274(15, C23H23O10), 443.0966(2.33E5; 100, C22H19O10), 295.0449(30, C13H11O8)
17.56	253.143	C14H21O4	235.1327(20, C14H19O3), 209.1535(5, C13H21O2), 191.1432(5.25E5; 100, C13H19O)
17.65	609.1597	C31H29O13	443.0955(5.44E5; 100, C22H19O10), 295.0442(3, C13H11O8)
17.73	487.123	C24H23O11	427.1014(5, C22H19O9), 367.0806(3, C20H15O7), 325.0703(10, C18H13O6), 297.0754(3, C17H13O5), 283.0600(5.80E5; 100, C16H11O5)
17.77	671.1769	C36H31O13	
17.81	242.1752	C13H24O3N	225.1490(60, C13H21O3), 181.1594(2.25E6; 100, C12H21O)

表2 ダイオウスペクトルリスト(Neg_8)

18.03	609.1613	C31H29O13	591.1476(35, C31H27O12), 443.0968(8.64E4; 100, C22H19O10), 295.0448(10, C13H11O8)
	329.2327	C18H33O5	329(50), 311.2219(35, C18H31O4), 293.2114(30, C18H29O3), 229.1438(2.95E5; 100, C12H21O4), 211.1334(70, C12H19O3), 183.1385(5, C11H19O2), 171.1022(15, C9H15O3)
18.12	449.1446	C22H25O10	389.1225(3, C20H21O8), 245.0810(1.08E6; 100, C14H13O4), 230.0577(5, C13H10O4)
	671.1766	C36H31O13	
18.16	581.1658	C30H29O12	
18.2	457.1138	C23H21O10	295.0601(10, C17H11O5), 277.0495(5, C17H9O4), 267.0651(3, C16H114), 253.0496(4.08E5; 100, C15H9O4)
18.25	296.1285	C18H18O3N	281.1048(8.91E5; 100, C17H15O3N)
18.38	457.114	C23H21O10	295.0602(10, C17H11O5), 277.0498(5, C17H9O4), 267.0654(3, C16H114), 253.0500(1.57E5; 100, C15H9O4)
	515.1921	C27H31O10	455.1698(3.33E5; 100, C25H27O8), 247.0969(3, C14H15O4), 163.0763(15, C10H11O2)
18.51	607.1819	C32H31O12	459.1277(7.18E5; 100, C23H23O10), 415.1382(3, C22H23O8)
	517.2077	C27H33O10	
18.55	229.1439	C12H21O4	229(50), 211.1335(7.07E5; 100, C12H19O3), 167.1439(45, C11H19O)
18.64	675.3746	C37H55O11	501.2833(7.03E3; 100, C29H41O7)
18.68	581.1661	C30H29O12	
18.81	329.1755	C20H25O4	285.1853(90, C19H25O2), 267.1747(20, C19H23O), 227.1435(4.71E4; 100, C16H19O), 209.1329(20, C16H17), 189.0916(20, C12H13O2)
18.94	256.1911	C14H26O3N	239.1647(50, C14H23O3), 195.1750(4.28E5; 100, C13H23O)
19.06	607.1811	C32H31O12	607(3.80E6; 100), 443.0970(80, C22H19O10), 295.0453(5, C13H11O8)
	721.1197	C38H25O13	693.0874(20, C36H21O15), 661.0982(3.79E5; 100, C36H21O13)
19.23	269.0448	C15H9O5	269(1.09E6; 100,), 240.0425(80, C14H8O4), 223.0399(3, C14H7O3)
19.35	283.0245	C15H7O6	283(40), 257.0450(80, C14H9O5), 243.0293(85, C13H7O5), 239.0347(1.75E6; 100, C14H7O4), 227.0347(50, C13H7O4), 215.0347(60, C12H7O4), 199.0399(30, C12H7O3), 187.0399(20, C11H7O3), 183.0451(10, C12H7O2), 155.0502(3, C11H7O)
19.56	607.182	C32H31O12	607(8.07E5; 100), 443.0966(50, C22H19O10), 295.0450(5, C13H11O8)
19.63	243.1591	C13H23O4	243(30), 225.1490(6.94E5; 100, C13H21O3), 181.1594(50, C12H21O)
22.26	269.0445	C15H9O5	269(1.07E6; 100,), 241.0498(10, C14H9O4), 225.0550(30, C14H9O3)

表3 サイコスペクトルリスト (1)

No.	Positive				Negative			
	保持時間 (min)	m/z (強度)	組成推定	Product Ions	保持時間 (min)	m/z (強度)	組成推定	Product Ions
1	5.7	205.0974 (8.15E7)	C11H13O2N2	188.0701(6.37E6; 100, C11H10O2N) 188 ⇒ 146.0595 (C9H8ON)	5.66	203.0816 (1.82E7)	C11H11O2N2	203(1.89E6; 100), 186.0553(10, C11H8O2N), 159.0922(98, C10H11N2), 142.0658(20, C10H8N), 116.0503(45, C8H6N)
2	7.62	217.0975 (2.09E7)	C12H13O2N2	171.0911(20, C11H11N2), 144.0802(2.09E6; 100, C10H10N)	7.5	215.0815 (7.49E6)	C12H11O2N2	215(50), 171.0921(7.03E5; 100, C11H11N2), 169.0767(30, C11H9N2), 142.0658(20, C10H8N), 116.0504(15, C8H6N)
3	9.06	355.1293 (2.67E7)	C19H19O5N2	232.0966(3.73E6; 100, C13H14O3N)	8.95	353.1136 (1.21E7)	C19H17O5N2	309.1231(6.59E6; 100, C18H17O3N2), 265.1335(5, C17H17ON2)
4	9.37	482.2589 (1.62E6)	C21H40O11N ([M+NH4] ⁺)	465.2330(15, C21H37O11), 447.2225(70, C21H35O10), 429.2119(70, C21H33O9), 333.1907(10, C16H29O7), 315.1800(40, C16H27O6), 297.1695(1.81E5; 100, C16H25O5), 295.1022(70, C11H19O9), 285.1694(50, C15H25O5), 267.1588(80, C15H23O4), 259.0809(20, C11H15O7), 153.1267(18, C10H17O9), 135.1162(25, C10H15)	9.35	523.2403 (2.89E7)	C23H39O13 ([M+AcO] ⁻)	463.2166([M-H] ⁻ , C21H35O11)
5	11.57	1107.5581 (2.88E6)	C53H87O24	1059.5378(25, C52H83O22), 927.4949(45, C47H75O18), 781.4365(1.43E4; 100, C41H65O14), 763.4255(45, C41H63O13)	11.58	612.2183, 2+ (2.26E7)	1165.5637, C55H89O26 ([M+AcO] ⁻)	612 → 851.4420(5, C44H67O16), 791.4207(10, C42H63O14), 582.2777(2- 2.40E5; 100, C55H88O26), 552.2673(60, C53H84O24), 313.1128(10, C22H42O20)
6	16.47	781.4734 (7.61E6)	C42H69O13	763.4623(15, C42H67O12), 745.4513(30, C42H65O11), 619.4199(10, C36H59O8), 601.4097(5, C36H57O7), 583.3990(5, C36H55O6), 455.3517(80, C30H47O3), 437.3413(1.79E5; 100, C30H45O2), 419.3307(25, C30H43O), 407.3308(15, C29H43O)	16.46	839.4787 (4.16E5)	C44H71O15 ([M+AcO] ⁻)	
7						857.4886 (2.17E7)	C44H73O16 ([M+AcO] ⁻)	797.4681 ([M-H] ⁻ , 1.01E4; 100, C42H69O14), 635.4153(15, C36H59O9)