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Mass Spectrum List Report

Analysis Info

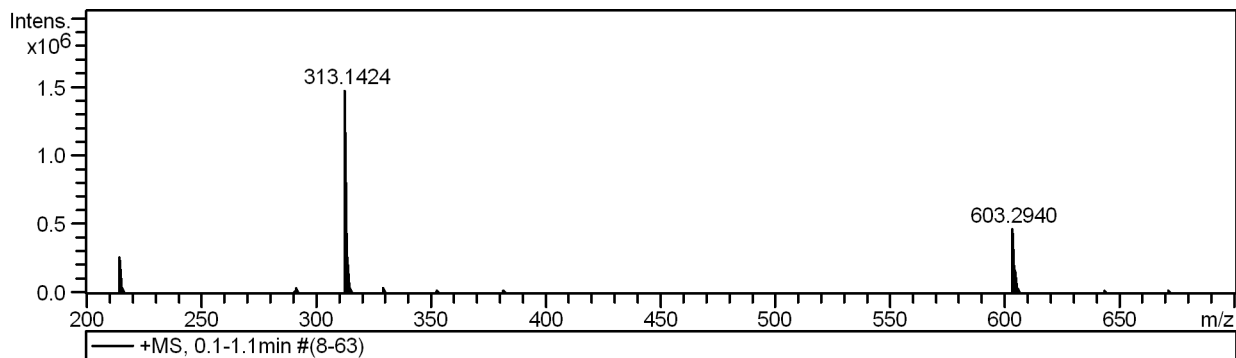
Analysis Name D:\Data\GuYL\gu-liu-20131218-1.d
Method tune_low.m
Sample Name gu-liu-20131218-1
Comment

Acquisition Date 12/18/2013 4:13:06 PM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	215.1071	4644	5834.8	261709	0.0463
2	313.1424	5039	22898.0	1482698	0.0621
3	603.2940	6200	8674.7	475180	0.0973

Mass Spectrum List Report

Analysis Info

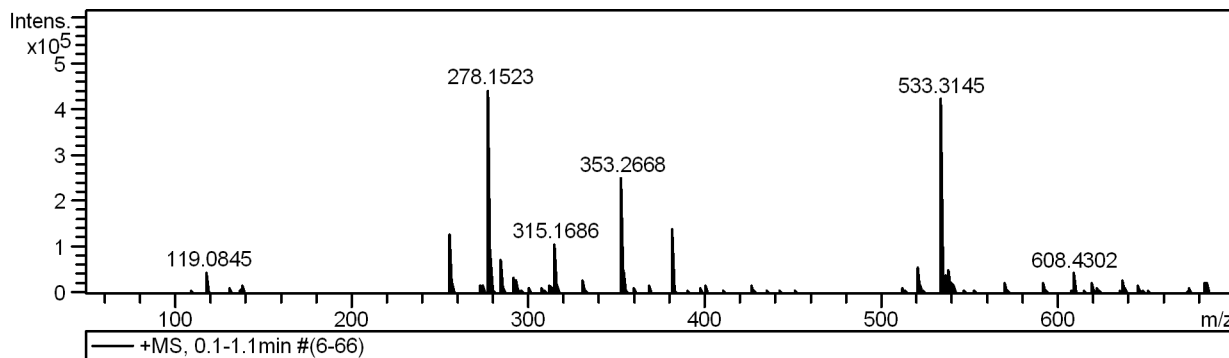
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Method tune_low.m
Sample Name gu-liu-20131218-2
Comment

Acquisition Date 12/18/2013 4:17:26 PM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	119.0845	4222	1539.3	47237	0.0282
2	256.1702	4985	1558.9	130559	0.0514
3	278.1523	5115	4712.4	443489	0.0544
4	315.1686	5391	973.3	108577	0.0585
5	353.2668	5424	1997.7	251960	0.0651
6	381.2982	5482	1082.1	142458	0.0696
7	533.3145	5953	2625.1	424342	0.0896
8	608.4302	5726	327.3	44538	0.1063

Mass Spectrum List Report

Analysis Info

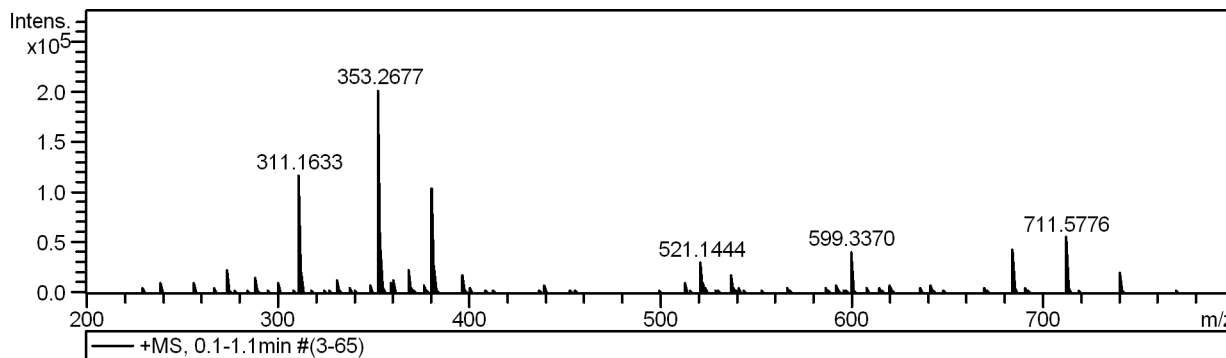
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Method tune_low.m
Sample Name gu-liu-20131218-03
Comment

Acquisition Date 12/18/2013 4:27:49 PM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	129.0549	4080	890.4	22799	0.0316
2	311.1633	5374	1902.4	117136	0.0579
3	353.2677	5493	2993.7	202453	0.0643
4	381.2993	5526	1568.5	104907	0.0690
5	521.1444	6132	493.5	31184	0.0850
6	599.3370	6236	640.9	41825	0.0961
7	683.5461	6497	634.6	43617	0.1052
8	711.5776	6434	793.3	55442	0.1106
9	739.6093	6611	295.6	20841	0.1119
10	949.8080	6808	352.3	18116	0.1395

Mass Spectrum List Report

Analysis Info

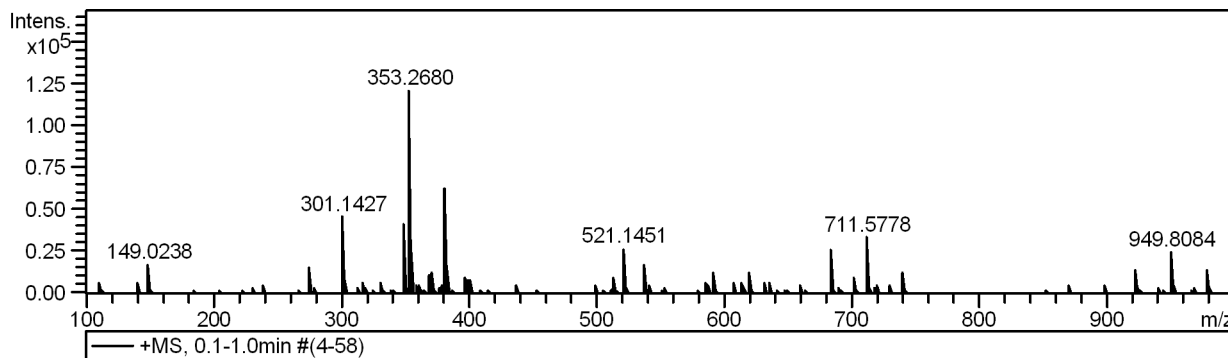
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Method tune_low.m
Sample Name gu-liu-20131218-04
Comment

Acquisition Date 12/18/2013 4:43:26 PM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	149.0238	4304	673.4	17474	0.0346
2	301.1427	5228	1034.5	45874	0.0576
3	348.9223	5457	861.2	42163	0.0639
4	353.2680	5523	2480.6	121161	0.0640
5	381.2995	5530	1302.1	62650	0.0690
6	521.1451	6100	609.1	27095	0.0854
7	683.5461	6457	536.6	25941	0.1059
8	711.5778	6442	678.4	33362	0.1105
9	921.7771	6931	277.1	14787	0.1330
10	949.8084	6688	474.8	24627	0.1420
11	977.8394	6635	291.1	14277	0.1474

Mass Spectrum List Report

Analysis Info

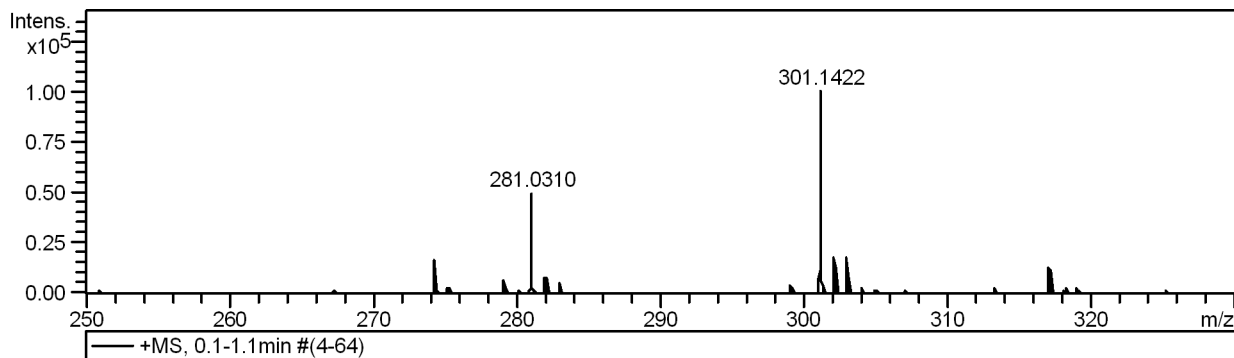
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Method tune_low.m
Sample Name gu-liu-20131218-05
Comment

Acquisition Date 12/18/2013 4:46:31 PM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	149.0235	4306	1023.0	28266	0.0346
2	281.0310	5106	1103.8	50075	0.0550
3	301.1422	5209	2097.3	100820	0.0578
4	353.2675	5501	1880.3	99466	0.0642
5	381.2987	5513	1012.8	52376	0.0692
6	591.4969	6124	279.4	12764	0.0966
7	633.2915	6042	332.6	15346	0.1048
8	683.5451	6510	416.8	19456	0.1050
9	711.5766	6435	545.6	25639	0.1106

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Analysis Info

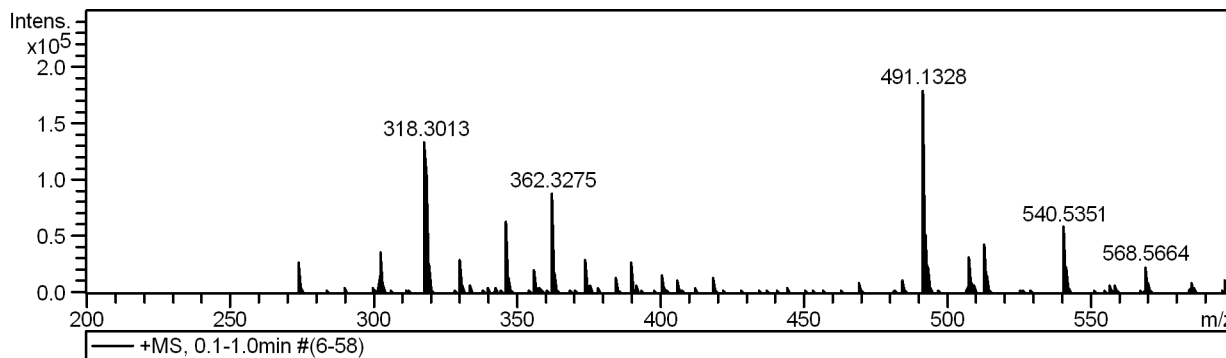
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Method tune_wide.m
Sample Name gu-liu-20131224-24
Comment

Acquisition Date 12/24/2013 10:44:34 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	274.2745	10366	517.5	28192	0.0265
2	302.3061	10724	604.9	37463	0.0282
3	318.3013	11235	2025.3	134005	0.0283
4	346.3321	10689	862.7	63237	0.0324
5	362.3275	10918	1152.6	88447	0.0332
6	374.3631	10330	381.7	30276	0.0362
7	390.3578	10569	349.7	28934	0.0369
8	491.1328	11964	1724.1	179917	0.0411
9	512.5036	10511	401.3	43716	0.0488
10	540.5351	10622	516.7	58778	0.0509
11	568.5664	10486	227.0	23988	0.0542

Mass Spectrum List Report

Analysis Info

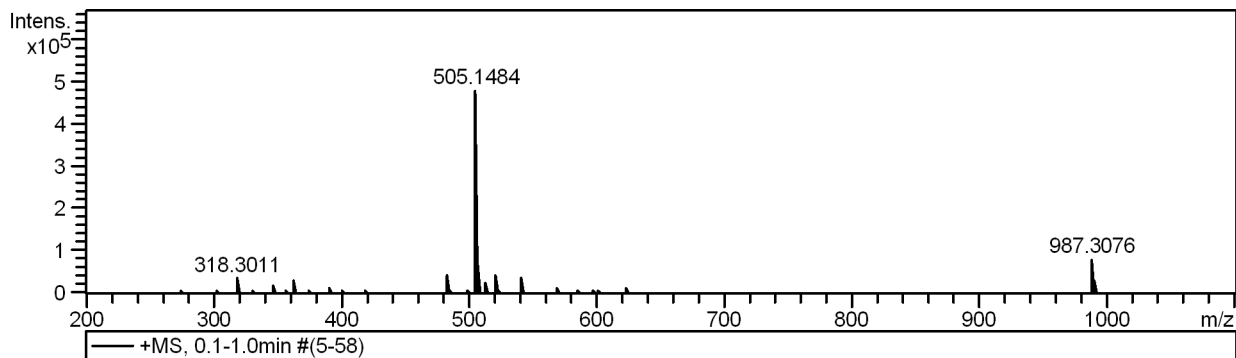
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Method tune_wide.m
Sample Name gu-liu-20131218-25
Comment

Acquisition Date 12/18/2013 10:33:02 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3011	10351	954.9	38115	0.0307
2	362.3275	10218	606.4	30028	0.0355
3	483.1657	10362	520.1	46220	0.0466
4	505.1484	13025	5016.3	481725	0.0388
5	521.1221	10309	454.9	46047	0.0506
6	540.5347	10110	339.5	35927	0.0535
7	987.3076	11930	1893.2	82707	0.0828

Mass Spectrum List Report

Analysis Info

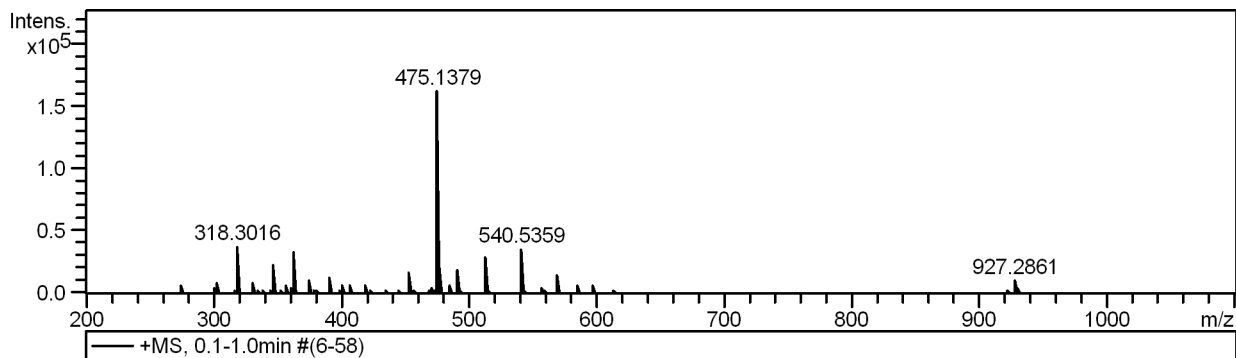
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Method tune_wide.m
Sample Name gu-liu-20131218-27
Comment

Acquisition Date 12/18/2013 10:38:32 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3016	10522	979.8	38635	0.0303
2	346.3329	10603	532.0	23040	0.0327
3	362.3280	10299	732.3	34156	0.0352
4	453.1573	10046	254.6	16697	0.0451
5	475.1379	11599	2322.8	162982	0.0410
6	512.5042	10478	372.4	29031	0.0489
7	540.5359	10210	441.4	36510	0.0529
8	568.5667	10443	182.0	14113	0.0544
9	927.2861	11199	283.2	11264	0.0828

Mass Spectrum List Report

Analysis Info

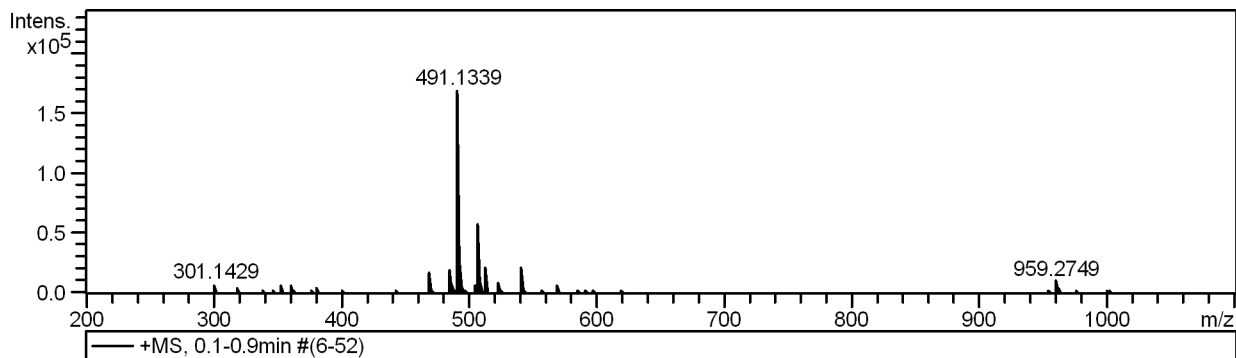
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Method tune_wide.m
Sample Name gu-liu-20131218-31
Comment

Acquisition Date 12/18/2013 10:43:12 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	301.1429	10357	227.0	7732	0.0291
2	469.1514	10432	260.0	18176	0.0450
3	491.1339	11756	2245.7	169512	0.0418
4	507.1204	9142	737.7	58672	0.0555
5	540.5360	10152	247.2	21439	0.0532
6	959.2749	10451	215.3	10338	0.0918
7	975.2620	9502	61.7	2870	0.1026

Mass Spectrum List Report

Analysis Info

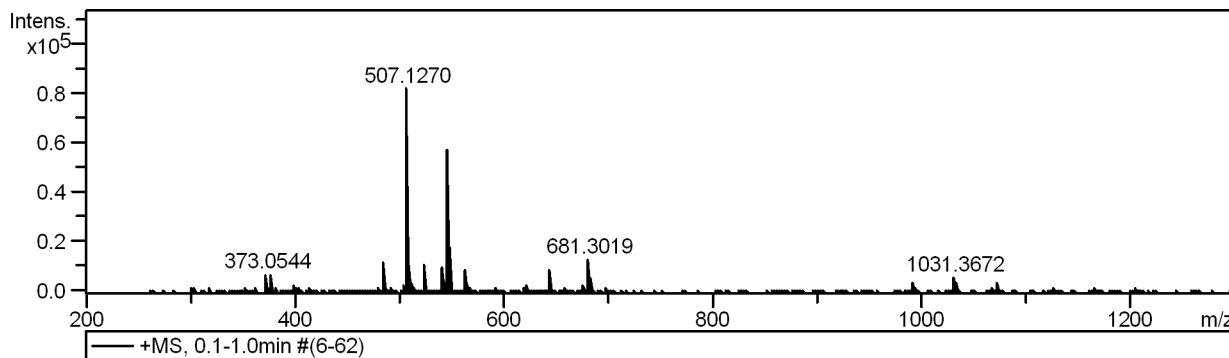
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Method tune_wide.m
Sample Name gu-liu-20131218-30
Comment

Acquisition Date 12/18/2013 10:47:33 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	373.0544	10497	306.2	7153	0.0355
2	377.0877	10023	298.0	7105	0.0376
3	485.1455	11140	317.6	11928	0.0435
4	507.1270	11755	2034.4	82088	0.0431
5	508.1301	10745	590.9	23918	0.0473
6	523.1060	9832	268.2	11365	0.0532
7	547.2302	11647	1325.3	57457	0.0470
8	643.1242	10783	249.3	8555	0.0596
9	681.3019	11492	424.7	13050	0.0593
10	991.2639	10823	158.7	4003	0.0916
11	1031.3672	10934	233.8	5966	0.0943

Mass Spectrum List Report

Analysis Info

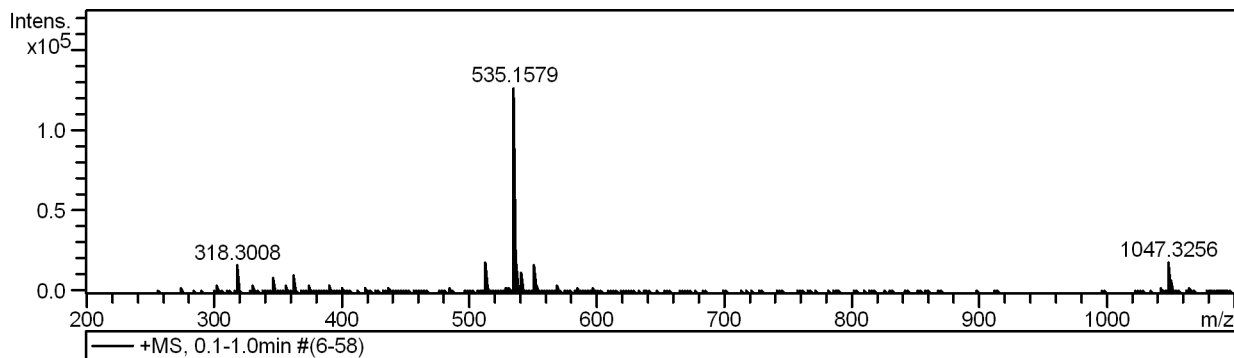
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Method tune_wide.m
Sample Name gu-liu-20131218-26
Comment

Acquisition Date 12/18/2013 10:51:16 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3008	10157	761.3	16377	0.0313
2	346.3320	10217	386.4	8983	0.0339
3	362.3271	10109	442.3	10962	0.0358
4	513.1763	10377	468.8	18398	0.0495
5	535.1579	11667	3059.8	126526	0.0459
6	551.1331	10790	427.9	17323	0.0511
7	1047.3256	10790	767.5	18117	0.0971

Mass Spectrum List Report

Analysis Info

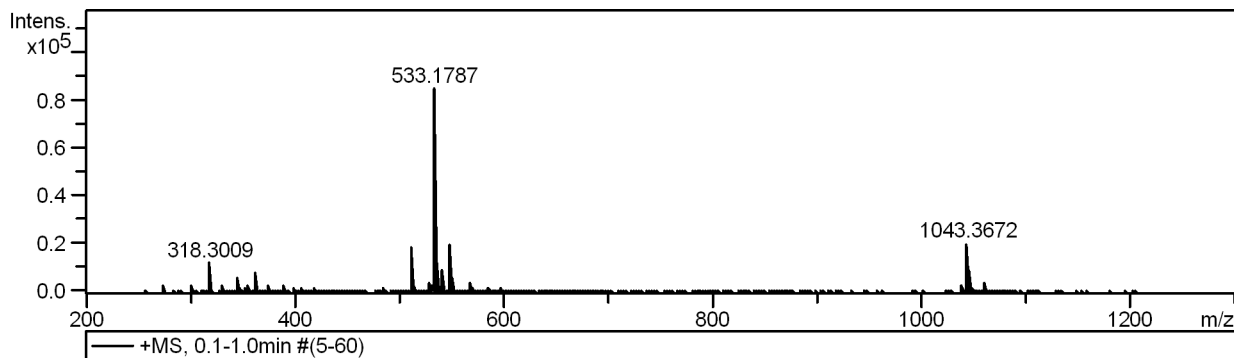
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Method tune_wide.m
Sample Name gu-liu-20131218-29
Comment

Acquisition Date 12/18/2013 10:55:36 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3009	10121	638.6	12086	0.0315
2	511.1968	10831	472.1	19171	0.0472
3	533.1787	10977	1963.2	84908	0.0486
4	549.1552	10621	473.0	20273	0.0517
5	1043.3672	10886	853.8	20196	0.0958

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Mass Spectrum List Report

Analysis Info

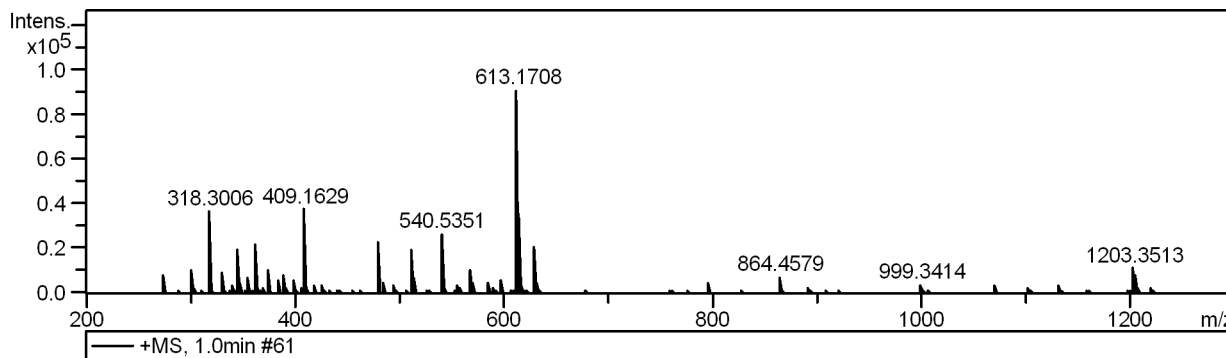
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Method tune_wide.m
Sample Name gu-liu-20131218-28
Comment

Acquisition Date 12/18/2013 10:59:27 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3006	10560	481.1	36768	0.0301
2	346.3323	10175	247.7	19709	0.0340
3	362.3274	10741	259.4	21700	0.0337
4	409.1629	10413	395.0	37783	0.0393
5	479.0947	11550	209.2	23760	0.0415
6	512.5029	10352	161.3	19697	0.0495
7	540.5351	11077	209.8	26927	0.0488
8	613.1708	10923	752.2	91101	0.0561
9	629.1456	10895	177.1	21164	0.0577
10	864.4579	9157	67.9	7676	0.0944
11	999.3414	11882	36.3	4168	0.0841
12	1203.3513	9782	114.8	11520	0.1230

Mass Spectrum List Report

Analysis Info

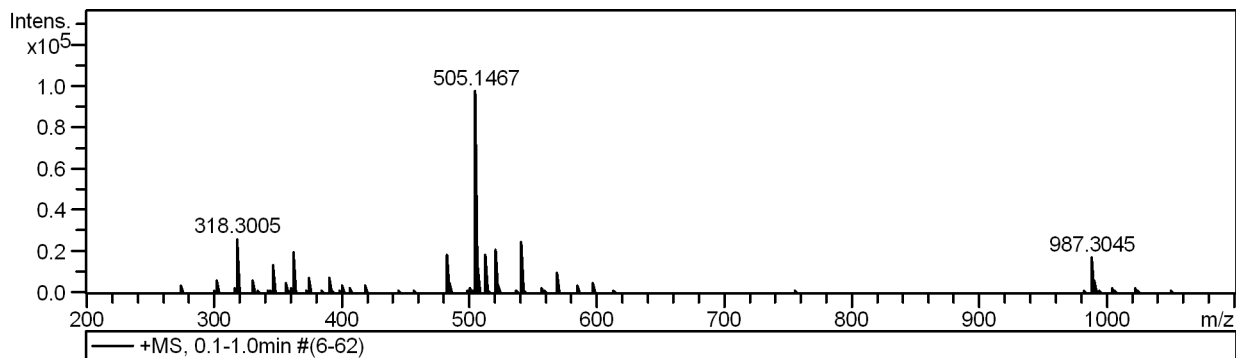
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Method tune_wide.m
Sample Name gu-liu-20131218-33
Comment

Acquisition Date 12/18/2013 11:03:44 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3005	10461	1003.7	26608	0.0304
2	346.3317	10120	499.7	14504	0.0342
3	362.3267	10222	646.4	20187	0.0354
4	483.1648	10296	400.7	19190	0.0469
5	505.1467	11298	1918.8	97714	0.0447
6	512.5022	10146	365.0	18960	0.0505
7	521.1263	9611	412.0	21889	0.0542
8	540.5336	10436	453.6	24991	0.0518
9	568.5654	10766	196.5	10164	0.0528
10	987.3045	11173	622.7	17437	0.0884

Mass Spectrum List Report

Analysis Info

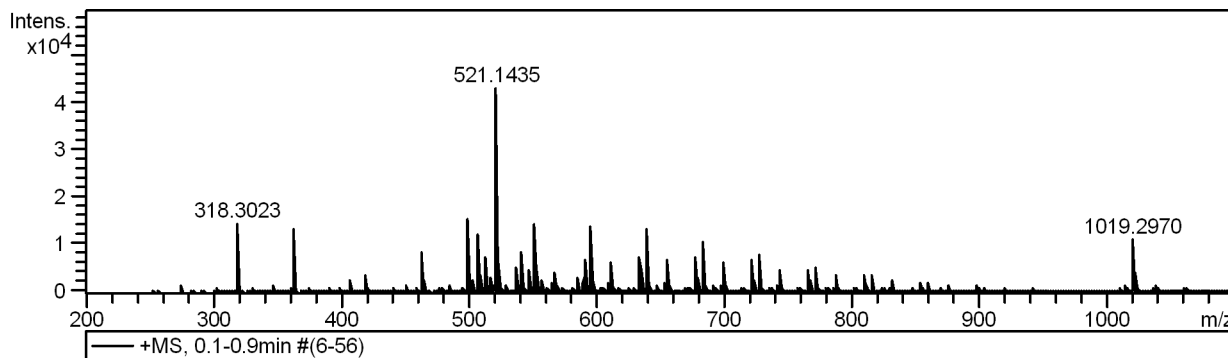
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Method tune_wide.m
Sample Name gu-liu-20131218-39
Comment

Acquisition Date 12/18/2013 11:09:01 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3023	10399	789.3	14392	0.0306
2	362.3284	9978	589.4	13376	0.0363
3	463.3042	10869	213.8	8377	0.0426
4	499.1620	10413	341.6	15386	0.0479
5	521.1435	10771	887.0	43135	0.0484
6	551.3568	11211	280.4	14344	0.0492
7	595.3826	10474	268.3	13556	0.0568
8	639.4084	11227	270.1	13473	0.0570
9	683.4344	10517	216.6	10665	0.0650
10	727.4614	11342	161.2	7834	0.0641
11	743.4362	10109	101.0	4831	0.0735
12	771.4870	10971	118.2	5384	0.0703
13	1019.2970	11291	391.8	10989	0.0903

Mass Spectrum List Report

Analysis Info

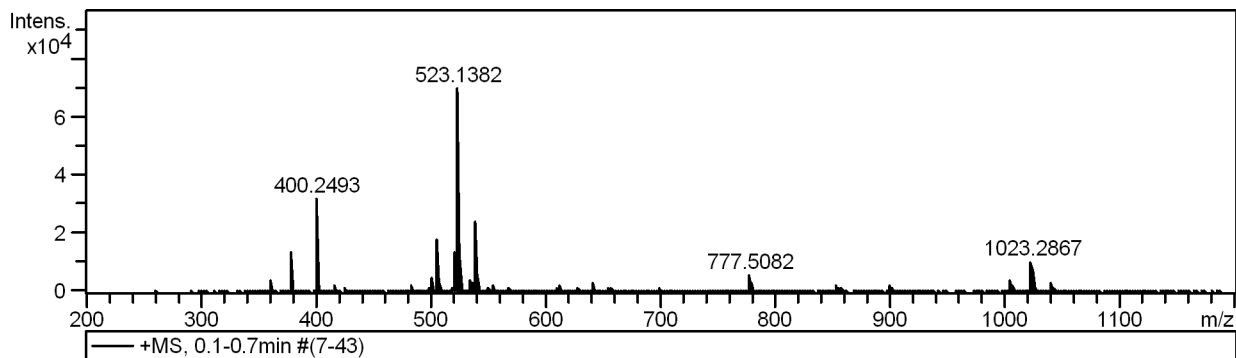
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Method tune_wide.m
Sample Name gu-liu-20131218-44-1
Comment

Acquisition Date 12/18/2013 11:18:09 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	378.2672	10988	482.9	13829	0.0344
2	400.2493	11562	1021.7	32096	0.0346
3	505.1476	11275	403.7	18133	0.0448
4	523.1382	11895	1485.0	70136	0.0440
5	539.1179	10095	492.8	24167	0.0534
6	777.5082	11149	153.8	5941	0.0697
7	1023.2867	11332	300.7	10478	0.0903

Mass Spectrum List Report

Analysis Info

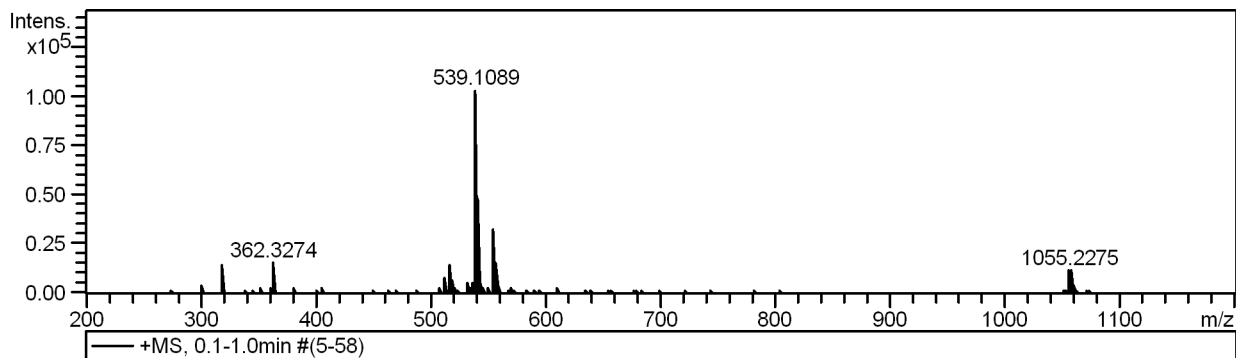
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Method tune_wide.m
Sample Name gu-liu-20131218-42
Comment

Acquisition Date 12/18/2013 11:21:54 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3014	10202	554.5	14934	0.0312
2	362.3274	10393	450.1	15414	0.0349
3	517.1269	10359	190.2	14211	0.0499
4	539.1089	11089	1288.6	102978	0.0486
5	555.0914	9650	427.9	33190	0.0575
6	1055.2275	10693	321.9	11784	0.0987

Mass Spectrum List Report

Analysis Info

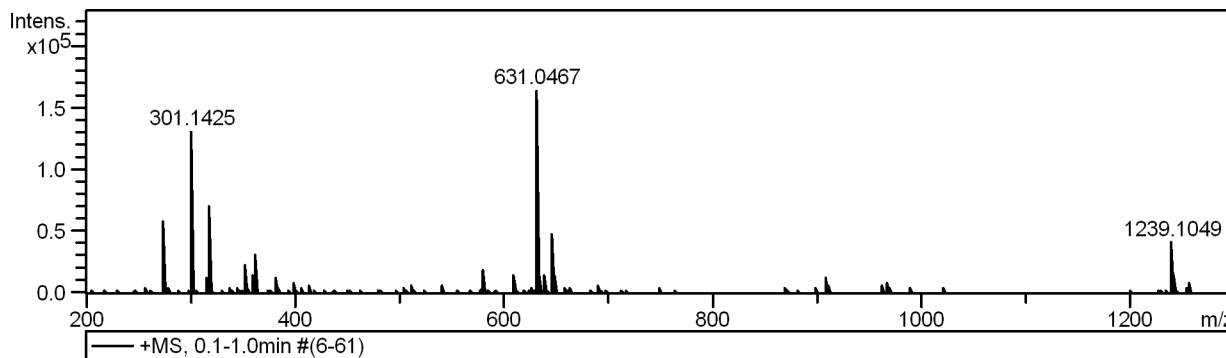
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Method tune_low.m
Sample Name gu-liu-20131218-47
Comment

Acquisition Date 12/18/2013 4:49:59 PM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	149.0237	4279	738.8	21126	0.0348
2	274.2756	5177	1217.6	58507	0.0530
3	301.1425	5217	2518.3	131559	0.0577
4	318.3019	5249	1301.3	71462	0.0606
5	362.3283	5480	546.0	32733	0.0661
6	631.0467	6349	2415.3	164928	0.0994
7	647.0279	6084	720.7	48714	0.1064
8	1239.1049	6920	1237.2	41734	0.1791

Mass Spectrum List Report

Analysis Info

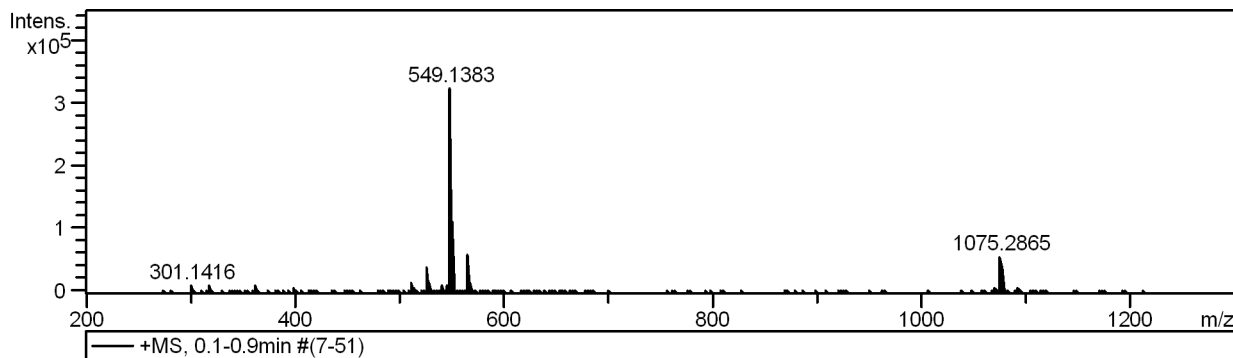
Analysis Name D:\Data\GuYL\gu-liu-20131218-54.d
Method tune_wide.m
Sample Name gu-liu-20131218-54
Comment

Acquisition Date 12/18/2013 11:29:54 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	301.1416	10636	437.6	11500	0.0283
2	527.1557	10638	525.5	38116	0.0496
3	549.1383	12693	4455.3	325039	0.0433
4	565.1134	10736	827.7	57982	0.0526
5	1075.2865	11800	1304.6	56438	0.0911

Mass Spectrum List Report

Analysis Info

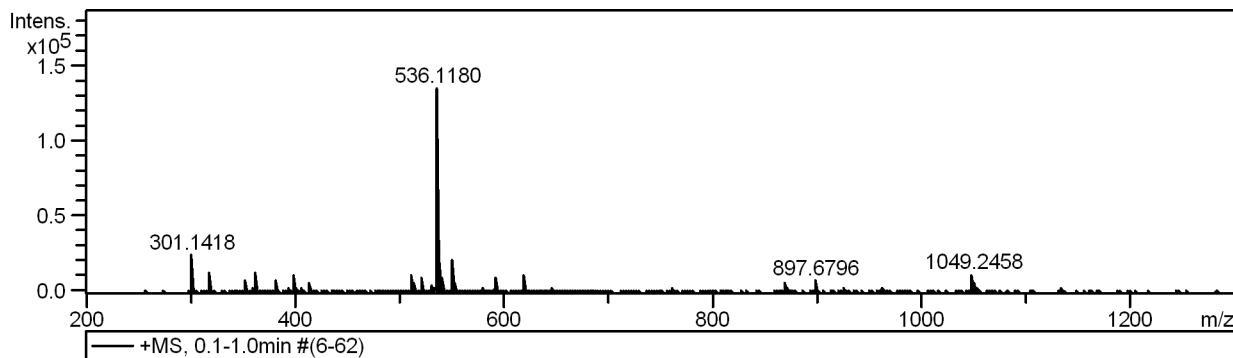
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Method tune_wide.m
Sample Name gu-liu-20131218-52
Comment

Acquisition Date 12/18/2013 11:34:14 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	301.1418	10268	1033.8	23969	0.0293
2	362.3280	10558	471.2	13654	0.0343
3	536.1180	11745	2531.5	135016	0.0456
4	552.0969	9678	404.1	21053	0.0570
5	897.6796	10404	227.9	7248	0.0863
6	1049.2458	10909	378.7	11288	0.0962

Mass Spectrum List Report

Analysis Info

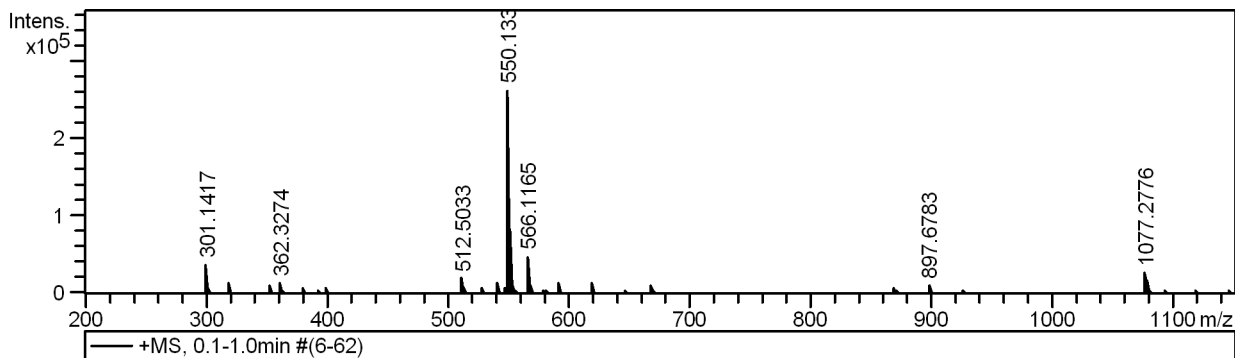
Analysis Name D:\Data\GuYL\gu-liu-20131218-53.d
Method tune_wide.m
Sample Name gu-liu-20131218-53
Comment

Acquisition Date 12/18/2013 11:37:18 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	301.1417	10564	1188.3	37820	0.0285
2	362.3274	10232	353.0	14228	0.0354
3	512.5033	10654	271.2	19951	0.0481
4	550.1336	12496	3405.4	263233	0.0440
5	566.1165	9753	648.7	48572	0.0580
6	897.6783	10480	237.1	10873	0.0857
7	1077.2776	11365	600.2	27280	0.0948

Mass Spectrum List Report

Analysis Info

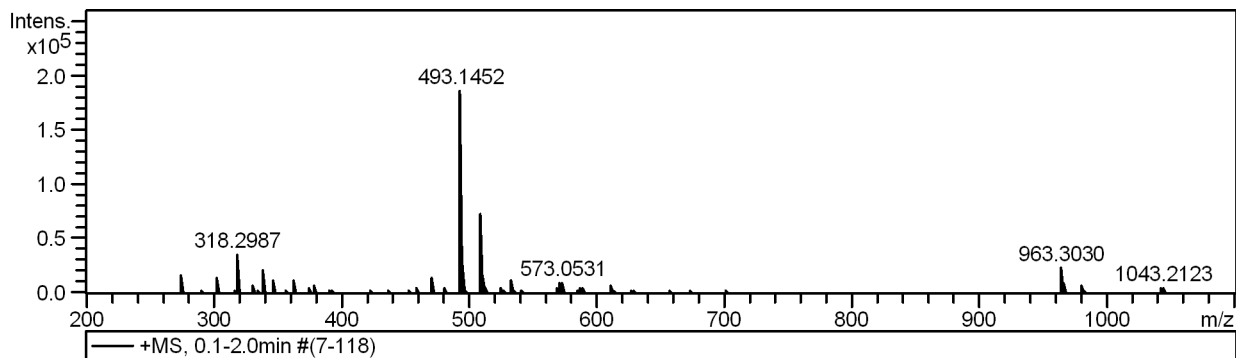
Analysis Name D:\Data\GuYL\gu20131011-2.d
Method tune_wide.m
Sample Name gu20131011-2
Comment

Acquisition Date 10/11/2013 11:13:43 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	274.2723	13138	613.1	17047	0.0209
2	318.2987	12309	1139.3	37066	0.0259
3	338.0982	11883	657.6	22770	0.0285
4	362.3243	11580	306.7	11900	0.0313
5	471.1630	12208	251.8	14734	0.0386
6	493.1452	13830	2998.5	187428	0.0357
7	509.1230	11878	1143.6	74792	0.0429
8	573.0531	12600	171.6	10879	0.0455
9	963.3030	12754	937.1	24645	0.0755
10	1043.2123	12064	243.9	6223	0.0865

Mass Spectrum List Report

Analysis Info

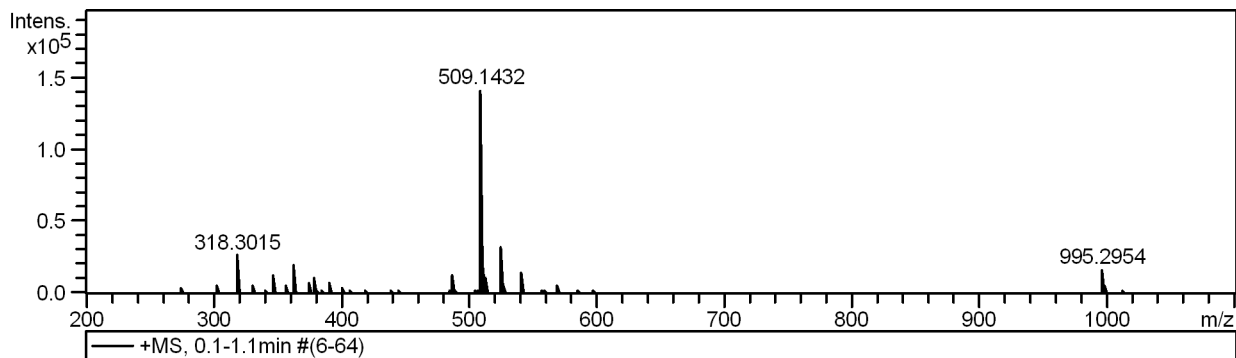
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Method tune_wide.m
Sample Name gu-liu-20131218-20
Comment

Acquisition Date 12/18/2013 11:40:38 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3015	10514	872.2	26796	0.0303
2	362.3271	10341	564.6	20211	0.0350
3	509.1432	11723	2537.4	141797	0.0434
4	525.1172	10535	558.0	32402	0.0498
5	540.5349	10721	261.7	15555	0.0504
6	995.2954	10907	592.1	16885	0.0913

Mass Spectrum List Report

Analysis Info

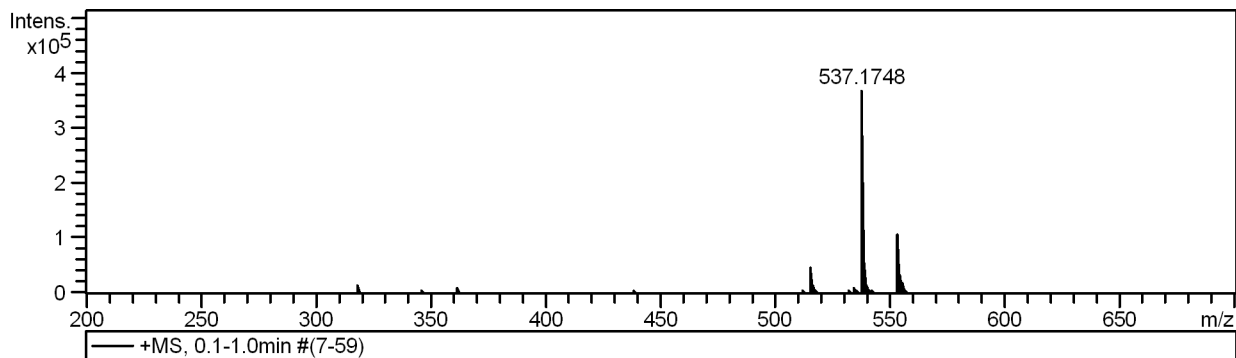
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Method tune_wide.m
Sample Name gu-liu-20131218-09
Comment

Acquisition Date 12/18/2013 11:45:23 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	515.1930	10590	737.6	49802	0.0486
2	537.1748	13081	5116.4	370154	0.0411
3	553.1486	11827	1547.7	107102	0.0468

Mass Spectrum List Report

Analysis Info

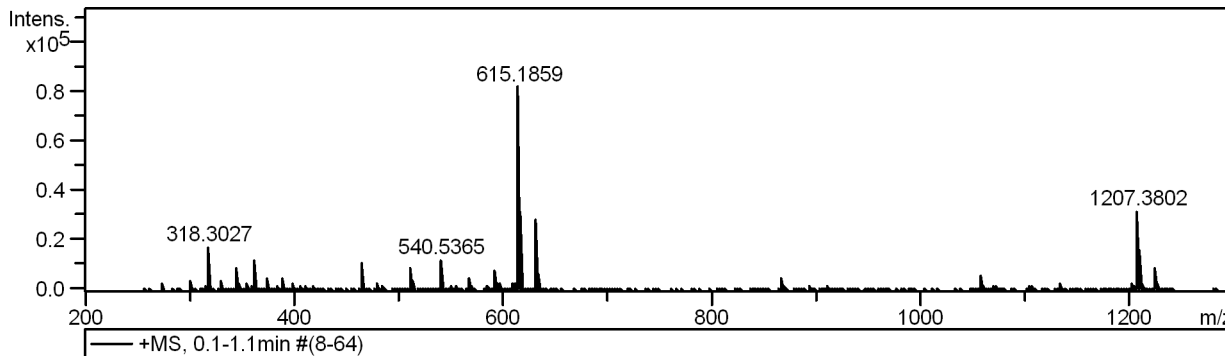
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Method tune_wide.m
Sample Name gu-liu-20131218-14
Comment

Acquisition Date 12/18/2013 11:48:43 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3027	10358	824.6	17211	0.0307
2	346.3336	9998	373.7	8488	0.0346
3	362.3286	10607	491.1	11971	0.0342
4	465.1359	10702	309.1	10840	0.0435
5	512.5042	10500	228.3	9130	0.0488
6	540.5365	10693	284.1	12041	0.0505
7	593.2042	10342	206.3	7756	0.0574
8	615.1859	11452	2293.6	81650	0.0537
9	631.1600	11448	840.7	28708	0.0551
10	1207.3802	11007	991.0	31774	0.1097

Mass Spectrum List Report

Analysis Info

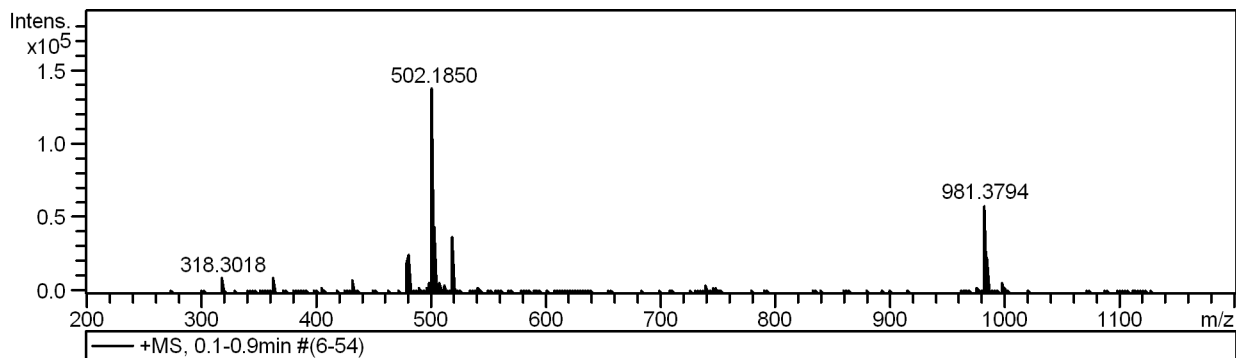
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Method tune_wide.m
Sample Name gu-liu-20131218-45
Comment

Acquisition Date 12/18/2013 11:54:37 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3018	10058	552.9	9526	0.0316
2	362.3279	10342	430.3	8999	0.0350
3	432.1995	10597	243.5	7302	0.0408
4	480.2035	10783	695.3	25191	0.0445
5	502.1850	11787	3526.3	137819	0.0426
6	518.1581	10914	892.0	36714	0.0475
7	981.3794	11634	2104.2	58750	0.0844

Mass Spectrum List Report

Analysis Info

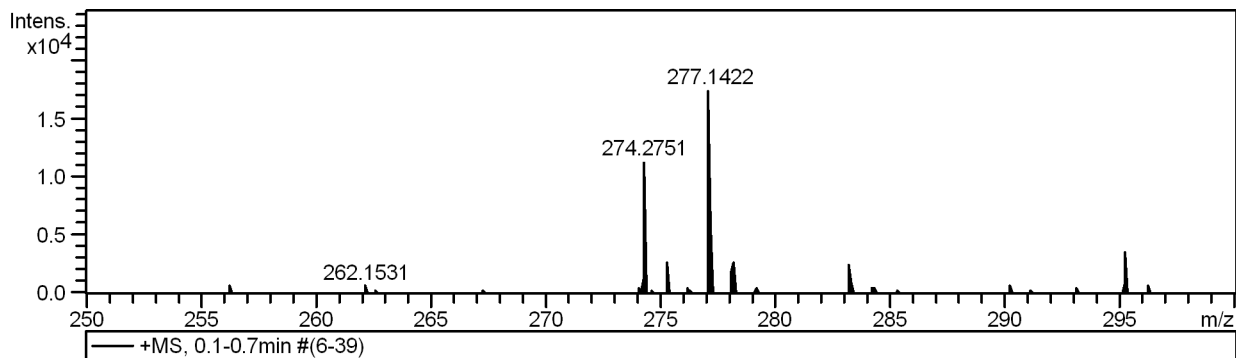
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Method tune_wide.m
Sample Name gu-liu-20140327-14
Comment

Acquisition Date 3/27/2014 10:22:39 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	262.1531	17132	16.4	674	0.0153
2	274.2751	11921	263.7	11376	0.0230
3	277.1422	17017	401.8	17498	0.0163

Mass Spectrum List Report

Analysis Info

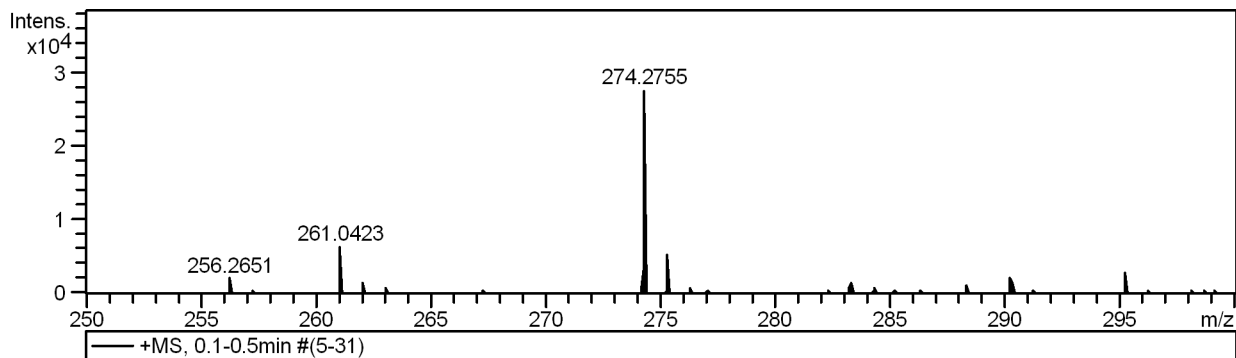
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Method tune_wide.m
Sample Name gu-liu-20140327-13
Comment

Acquisition Date 3/27/2014 10:18:29 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	256.2651	12792	25.8	2060	0.0200
2	261.0423	12410	78.4	6407	0.0210
3	262.0465	15544	17.0	1398	0.0169
4	263.0398	11309	7.8	644	0.0233
5	263.0398	11309	7.8	644	0.0233
6	274.2755	12201	317.0	27683	0.0225
7	275.2785	12410	62.0	5441	0.0222

Mass Spectrum List Report

Analysis Info

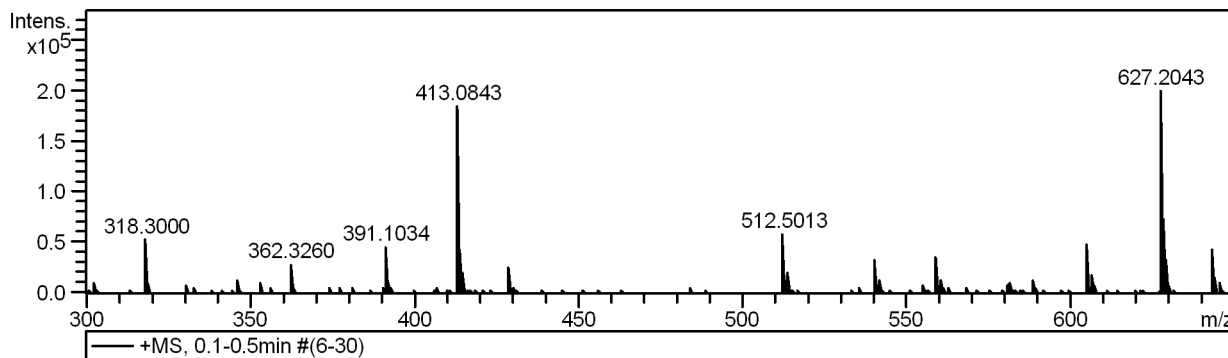
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Method tune_wide.m
Sample Name gu-liu-20140327-10
Comment

Acquisition Date 3/27/2014 10:09:16 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3000	13228	649.3	53355	0.0241
2	362.3260	14312	307.1	29866	0.0253
3	391.1034	16223	427.6	46272	0.0241
4	413.0843	16401	1588.5	185278	0.0252
5	512.5013	17009	383.0	59175	0.0301
6	627.2043	16041	1604.6	200676	0.0391

Mass Spectrum List Report

Analysis Info

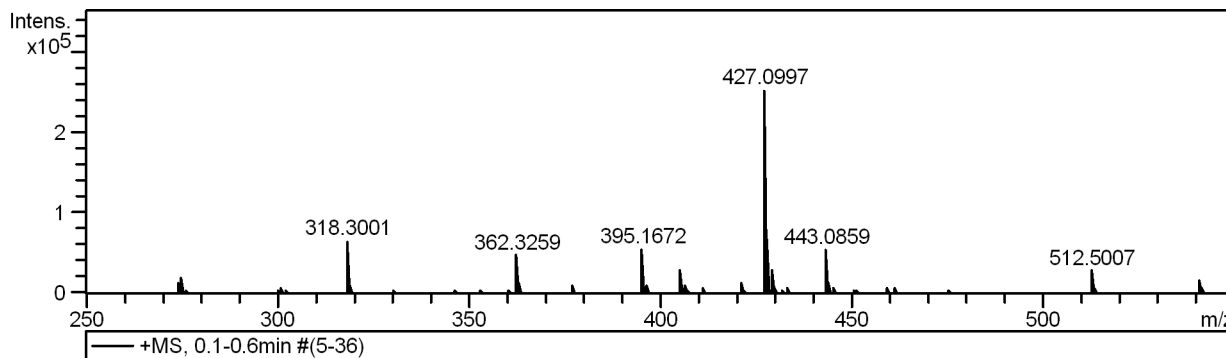
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Method tune_wide.m
Sample Name gu-liu-20140327-1
Comment

Acquisition Date 3/27/2014 9:42:55 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3001	17112	837.0	66140	0.0186
2	362.3259	14521	540.3	47415	0.0250
3	395.1672	17107	612.5	55808	0.0231
4	405.1186	15368	315.0	29020	0.0264
5	427.0997	14991	2681.4	252923	0.0285
6	443.0859	10701	569.2	54641	0.0414
7	512.5007	16555	275.8	28427	0.0310

Mass Spectrum List Report

Analysis Info

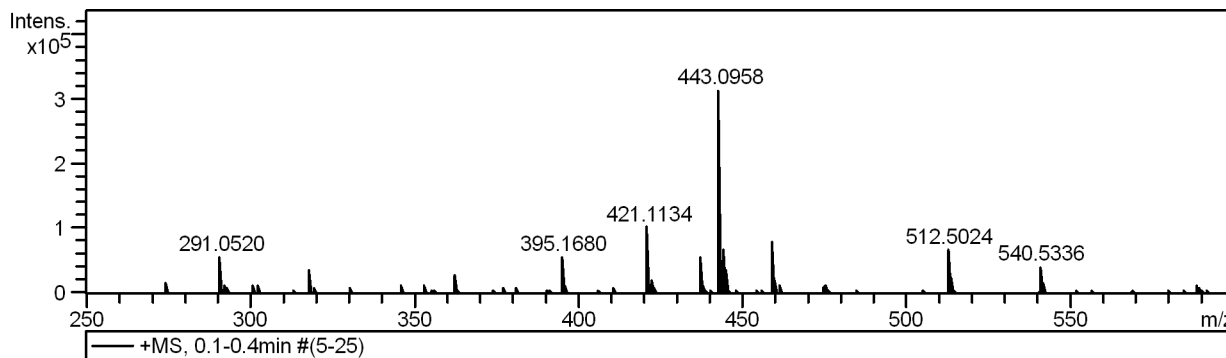
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Method tune_wide.m
Sample Name gu-liu-20140327-11
Comment

Acquisition Date 3/27/2014 10:11:48 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	291.0520	12208	684.4	57114	0.0238
2	395.1680	13471	492.5	57209	0.0293
3	421.1134	17554	826.8	102680	0.0240
4	443.0958	16758	2403.0	314892	0.0264
5	459.0827	10885	594.1	80777	0.0422
6	512.5024	16171	446.6	68112	0.0317
7	540.5336	16289	265.0	42328	0.0332

Mass Spectrum List Report

Analysis Info

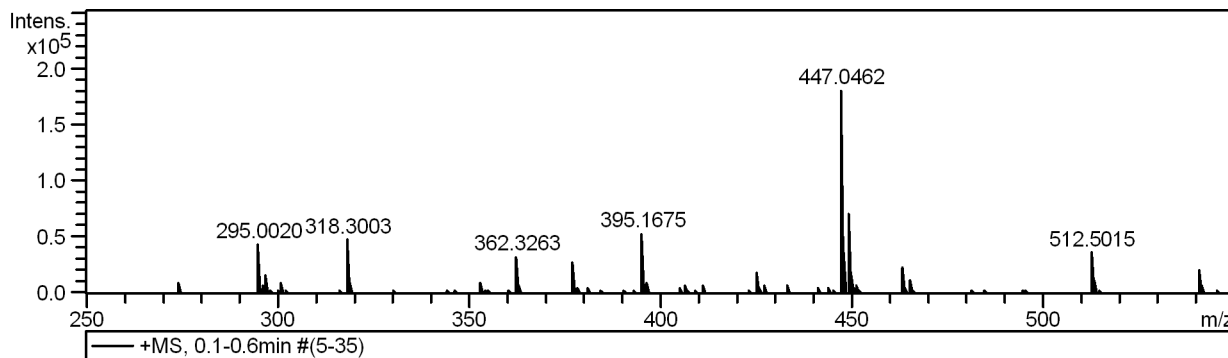
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Method tune_wide.m
Sample Name gu-liu-20140327-5-1
Comment

Acquisition Date 3/27/2014 9:57:06 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	295.0020	16840	701.1	44360	0.0175
2	318.3003	14479	700.3	48056	0.0220
3	362.3263	13303	420.6	33545	0.0272
4	395.1675	15163	604.7	53752	0.0261
5	447.0462	17854	1759.3	181563	0.0250
6	512.5015	17856	305.6	37141	0.0287

Mass Spectrum List Report

Analysis Info

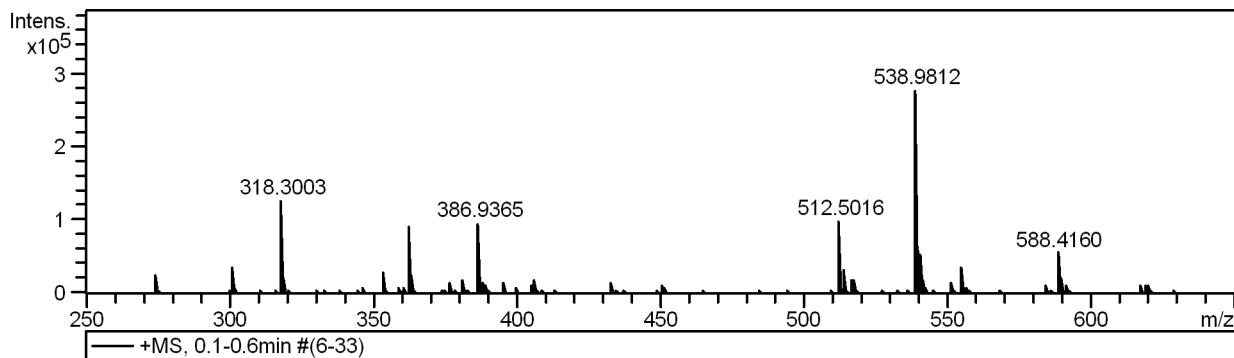
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Method tune_wide.m
Sample Name gu-liu-20140327-2
Comment

Acquisition Date 3/27/2014 9:46:12 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3003	16067	1245.8	127199	0.0198
2	362.3264	14145	756.6	92387	0.0256
3	386.9365	14984	723.0	97022	0.0258
4	512.5016	17822	508.3	99567	0.0288
5	538.9812	17318	1336.3	278539	0.0311
6	588.4160	16101	299.4	56114	0.0365

Mass Spectrum List Report

Analysis Info

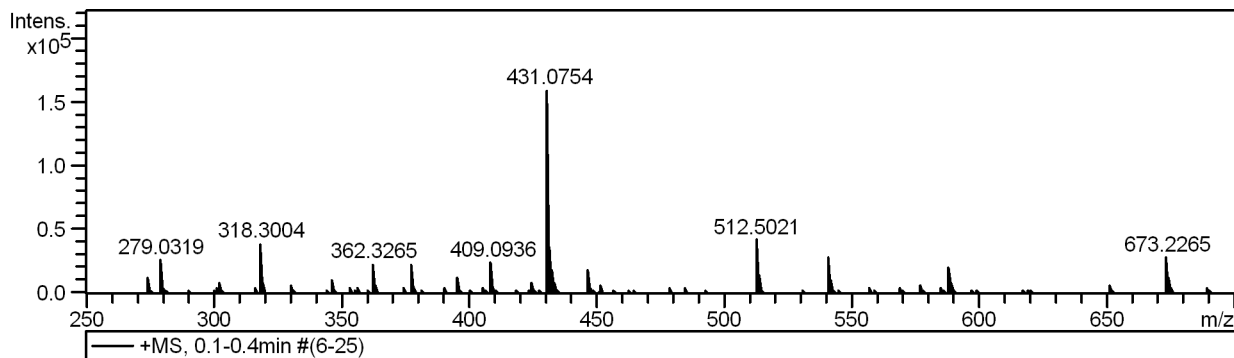
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Method tune_wide.m
Sample Name gu-liu-20140327-6
Comment

Acquisition Date 3/27/2014 9:59:50 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	279.0319	16031	401.3	26696	0.0174
2	318.3004	13997	519.1	39757	0.0227
3	362.3265	13500	276.4	23492	0.0268
4	409.0936	15820	269.5	24412	0.0259
5	431.0754	14887	1714.2	159894	0.0290
6	512.5021	17171	408.4	42068	0.0298
7	673.2265	15826	340.2	28684	0.0425

Mass Spectrum List Report

Analysis Info

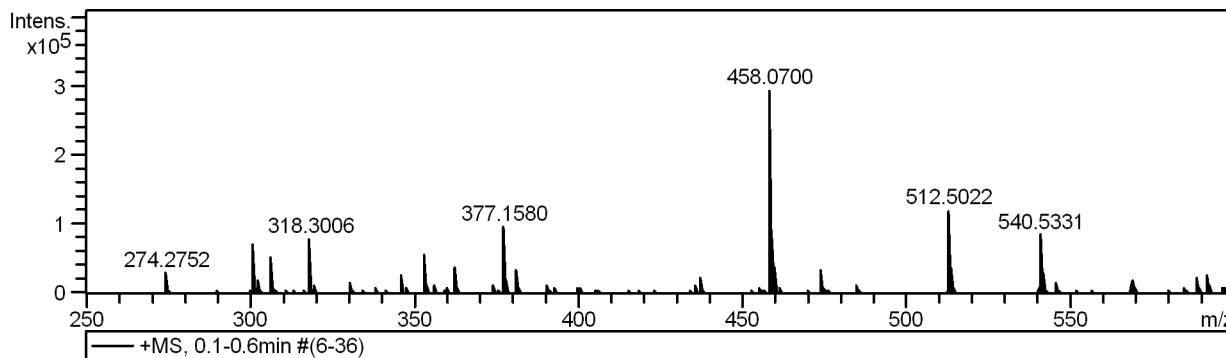
Analysis Name D:\Data\GuYL\gu-liu-20140327-3.d
Method tune_wide.m
Sample Name gu-liu-20140327-3
Comment

Acquisition Date 3/27/2014 9:49:33 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	274.2752	16285	355.8	30452	0.0168
2	301.1417	16801	734.1	71256	0.0179
3	318.3006	15267	759.7	79324	0.0208
4	377.1580	16017	751.0	96758	0.0235
5	458.0700	15381	1821.8	294882	0.0298
6	512.5022	18239	656.0	120684	0.0281
7	540.5331	16152	441.3	85354	0.0335

Mass Spectrum List Report

Analysis Info

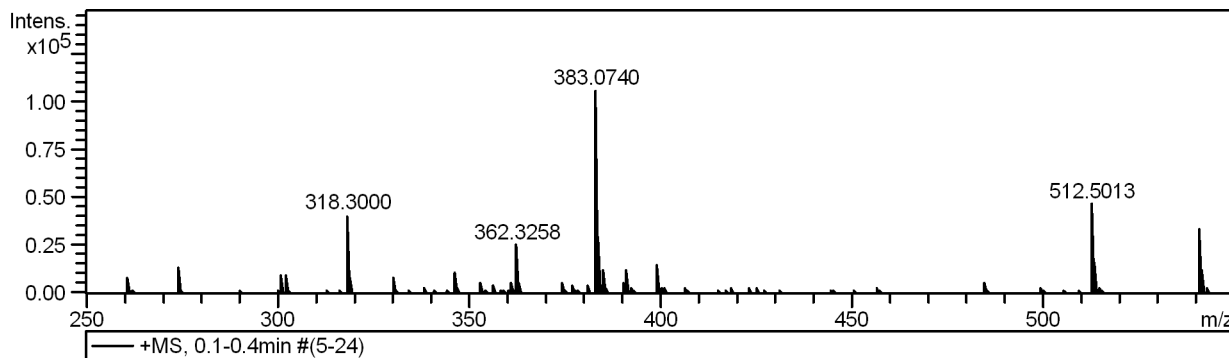
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Method tune_wide.m
Sample Name gu-liu-20140327-8
Comment

Acquisition Date 3/27/2014 10:04:30 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3000	13717	580.8	40870	0.0232
2	362.3258	13523	326.8	25132	0.0268
3	383.0740	13428	1354.5	106107	0.0285
4	512.5013	17084	535.0	46568	0.0300
5	540.5322	15920	381.1	33799	0.0340

Mass Spectrum List Report

Analysis Info

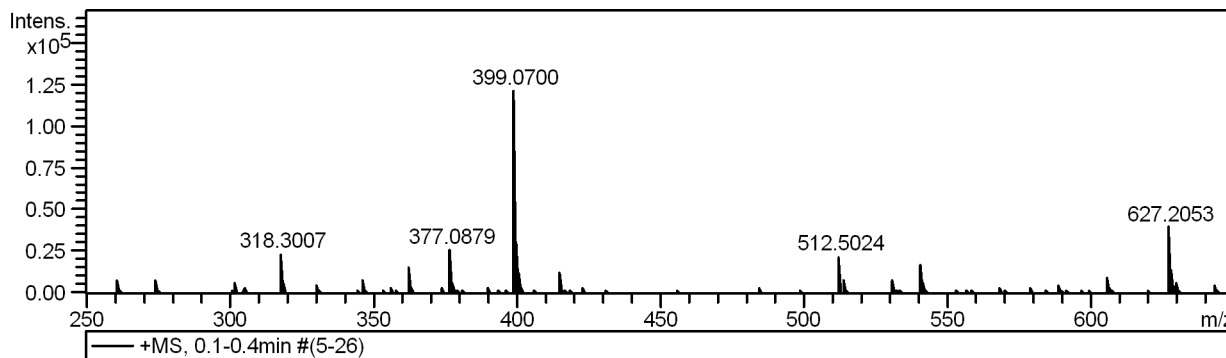
Analysis Name D:\Data\GuYL\gu-liu-20140327-12.d
Method tune_wide.m
Sample Name gu-liu-20140327-12
Comment

Acquisition Date 3/27/2014 10:15:14 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3007	12553	419.9	24059	0.0254
2	362.3267	14840	257.5	16020	0.0244
3	377.0879	15394	416.7	26349	0.0245
4	399.0700	14320	1883.2	121952	0.0279
5	512.5024	16010	313.3	22718	0.0320
6	627.2053	15065	612.1	39942	0.0416

Mass Spectrum List Report

Analysis Info

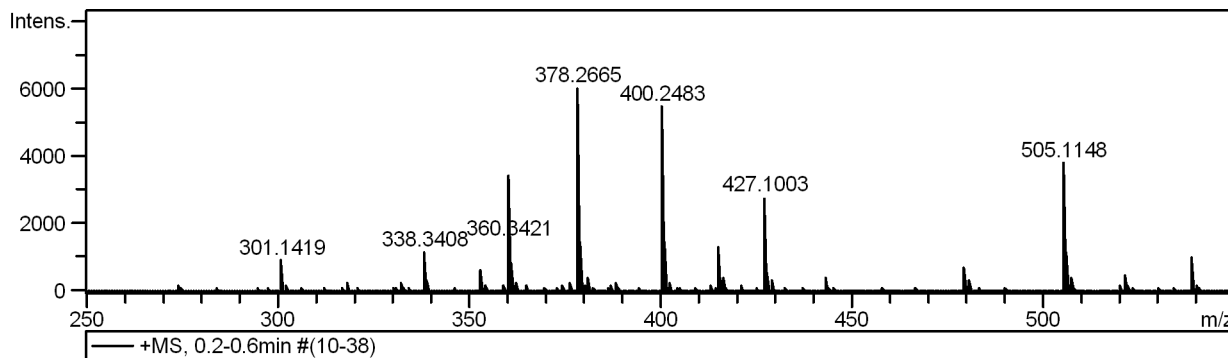
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Method tune_wide.m
Sample Name gu-liu-20140327-5
Comment

Acquisition Date 3/27/2014 9:55:00 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	301.1419	16411	69.3	919	0.0184
2	338.3408	13983	80.5	1174	0.0242
3	360.3421	4576	99.5	1493	0.0787
4	378.2665	15993	394.1	6034	0.0237
5	400.2483	14637	349.7	5485	0.0273
6	427.1003	16063	172.8	2789	0.0266
7	505.1148	16583	217.2	3804	0.0305
8	538.9814	18039	54.8	989	0.0299

Mass Spectrum List Report

Analysis Info

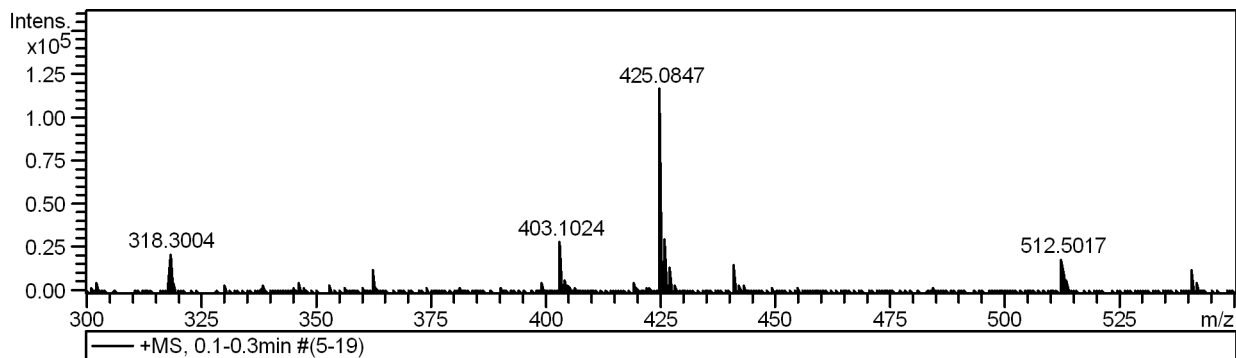
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Method tune_wide.m
Sample Name gu-liu-20140327-7
Comment

Acquisition Date 3/27/2014 10:02:18 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.3004	14051	340.5	21910	0.0227
2	403.1024	14839	402.1	29024	0.0272
3	425.0847	14858	1585.2	116715	0.0286
4	512.5017	16822	239.4	19056	0.0305

Mass Spectrum List Report

Analysis Info

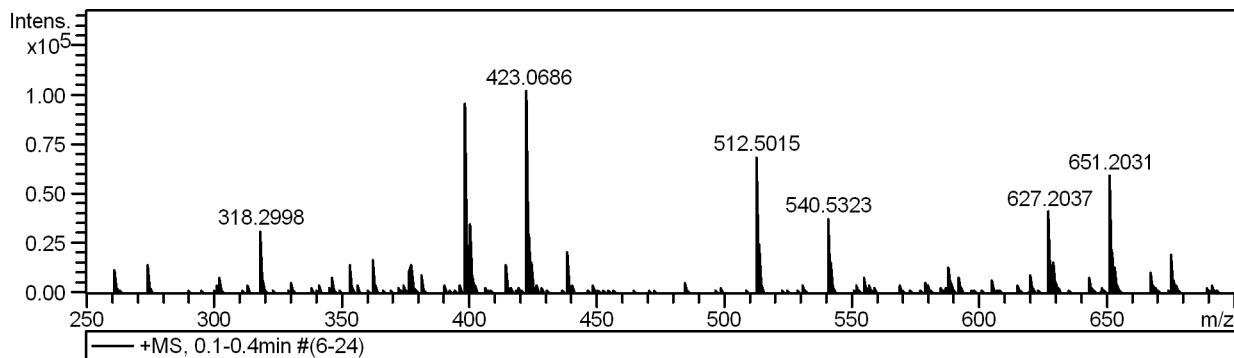
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Method tune_wide.m
Sample Name gu-liu-20140327-9
Comment

Acquisition Date 3/27/2014 10:07:01 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	318.2998	13334	364.8	31915	0.0239
2	423.0686	13846	915.0	102520	0.0306
3	512.5015	16963	524.0	68728	0.0302
4	540.5323	15526	278.8	37992	0.0348
5	627.2037	15922	350.7	41193	0.0394
6	651.2031	16400	529.2	59404	0.0397

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Mass Spectrum List Report

Analysis Info

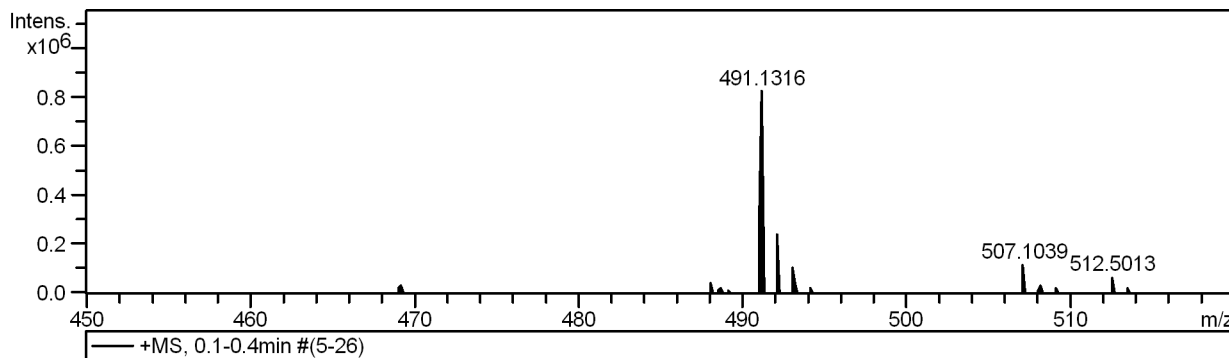
Analysis Name D:\Data\GuYL\gu-liu-20140327-16.d
Method tune_wide.m
Sample Name gu-liu-20140327-16
Comment

Acquisition Date 3/27/2014 3:47:56 PM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	3.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	488.1244	15762	286.6	41229	0.0310
2	491.1316	19043	5680.3	826492	0.0258
3	492.1337	16698	1696.6	247745	0.0295
4	493.1290	14382	720.9	105657	0.0343
5	507.1039	15978	775.4	119455	0.0317
6	512.5013	15729	451.0	70783	0.0326

Analysis Info

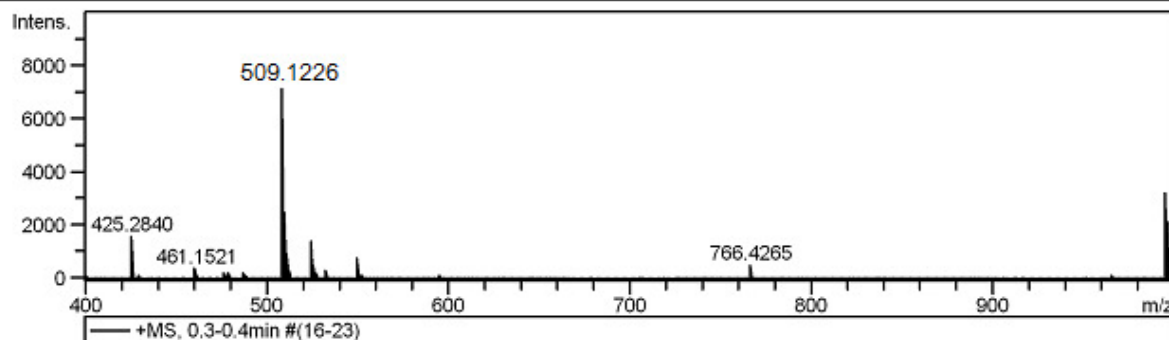
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Method tune_wide.m
Sample Name gu-liu-20140625-4-1
Comment

Acquisition Date 6/25/2014 10:00:56 AM

Operator BDAL@DE
Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	425.2840	17523	183.0	1590	0.0243
2	461.1521	19455	41.2	392	0.0237
3	509.1226	14342	684.5	7271	0.0355
4	510.1403	14899	238.2	2536	0.0342
5	511.1374	12590	88.1	940	0.0406
6	525.1106	14433	132.3	1454	0.0364
7	550.1632	14482	68.2	759	0.0380
8	766.4265	39757	61.0	528	0.0193
9	995.2849	16841	355.2	3236	0.0591

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
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Mass Spectrum List Report

Analysis Info

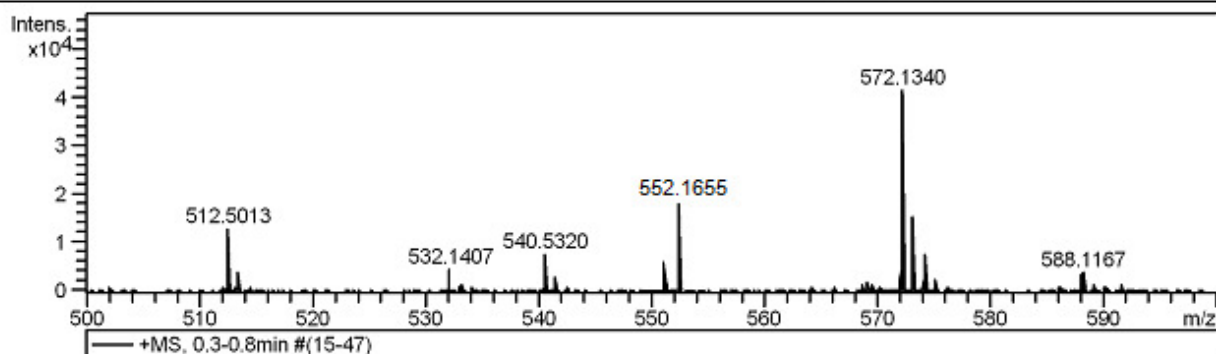
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 Method tune_low.m
 Sample Name gu-liu-20140715-1
 Comment

Acquisition Date 7/15/2014 3:13:05 PM

Operator BDAL@DE
 Instrument / Ser# micrOTOF 10401

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active			Set Dry Heater	180 °C
Scan Begin	50 m/z	Set Capillary	4500 V	Set Dry Gas	4.0 l/min
Scan End	3000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	FWHM
1	512.5013	15901	438.5	12923	0.0322
2	532.1407	16034	145.9	4553	0.0332
3	540.5320	14869	242.5	7659	0.0364
4	552.1655	15214	586.5	18135	0.0362
5	572.1340	15694	1415.9	41627	0.0365
6	572.1340	15694	1415.9	41627	0.0365
7	573.1368	15421	520.9	15278	0.0372
8	574.1326	13945	253.3	7410	0.0412
9	588.1167	11246	138.7	3924	0.0523

Meas. m/z	#	Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
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