

Supporting Information 2

Optimization of tetrahydroindazoles as inhibitors of human dihydroorotate dehydrogenase and evaluation of their activity and in vitro metabolic stability

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**corresponding author*

Content of Supporting Information:

Supporting Information 1:

Supplementary Figures S1 – S14.

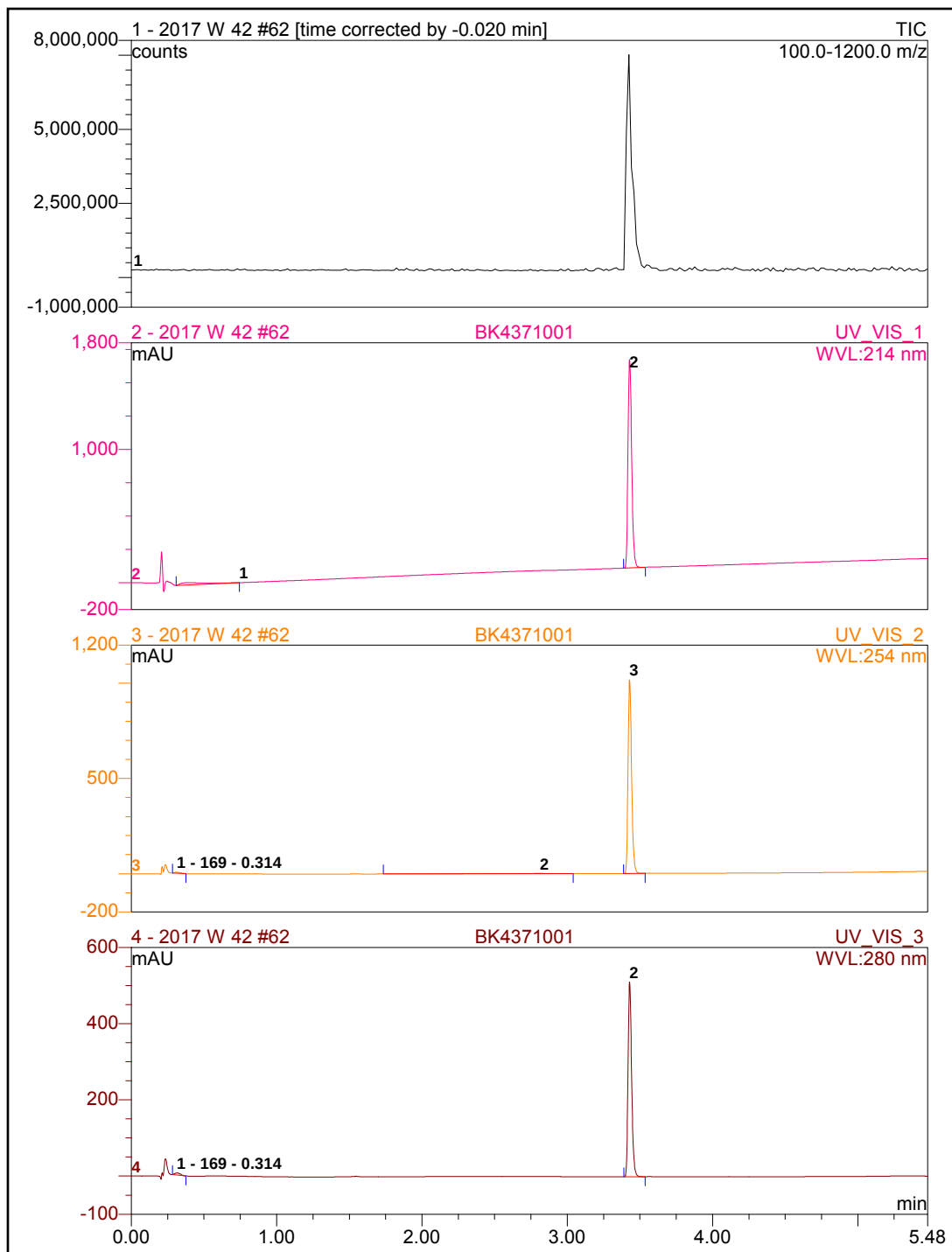
Supplementary Tables S1 - S3.

Supporting Information 2:

A pdf file containing the HPLC and HRMS raw data of selected compounds.

Supporting Information 3:

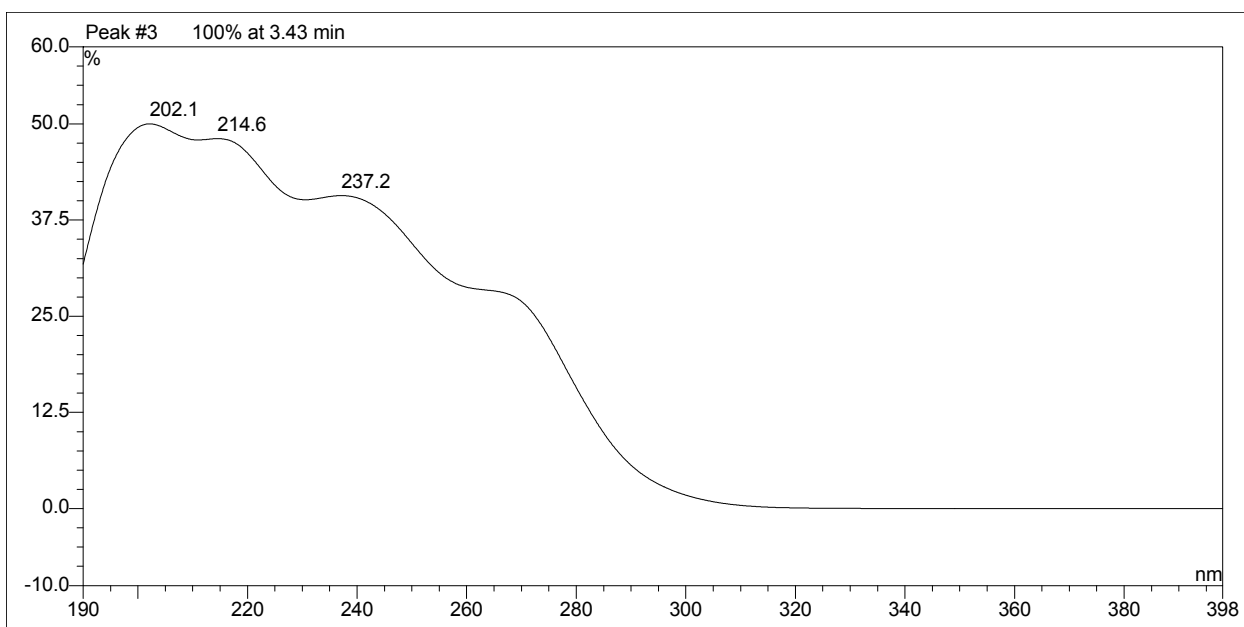
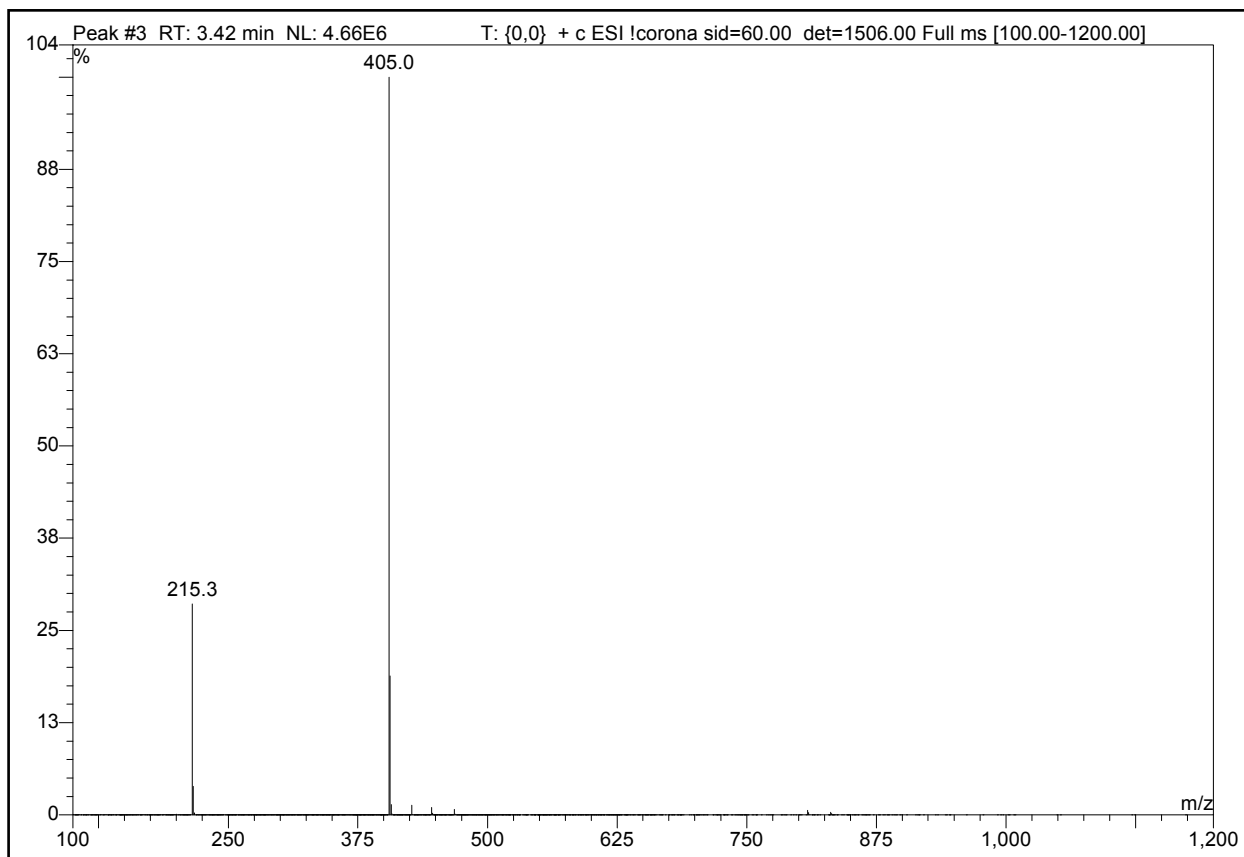
Molecular formula strings table.

Compound 30**Sample Name:** BK4371001**Injection Volume:** 5.0 uL**Control Program:** Purity 5 min 5-100% positive**UserID** UY**Recording Time:** 10/17/2017 11:06**Highest m/z responses**

No.	Ret.Time min	Height mAU	Area mAU*min	Rel.Area %	Mass - 1 m/z	Mass - 2 m/z	Mass - 3 m/z
1	0.31	5.332	0.236	0.79	134	114	108
2	2.81	1.528	0.944	3.17	115	167	103
3	3.43	1017.153	28.638	96.04	405	215	406

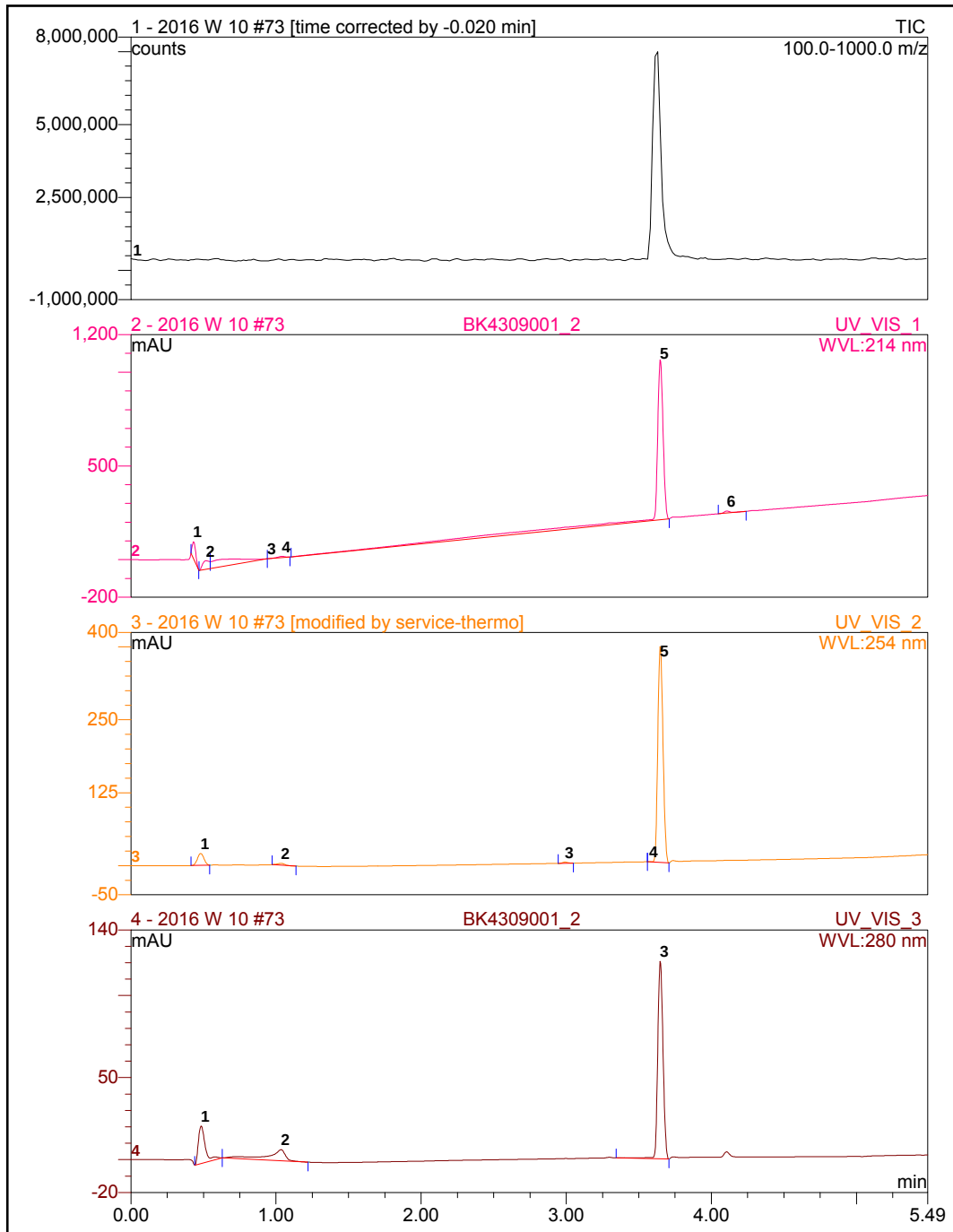
Sample Name: BK4371001
Control Program Purity 5 min 5-100% positive
Recording Time:#####

Injection Volume: 5.0 μ L
UserID UY



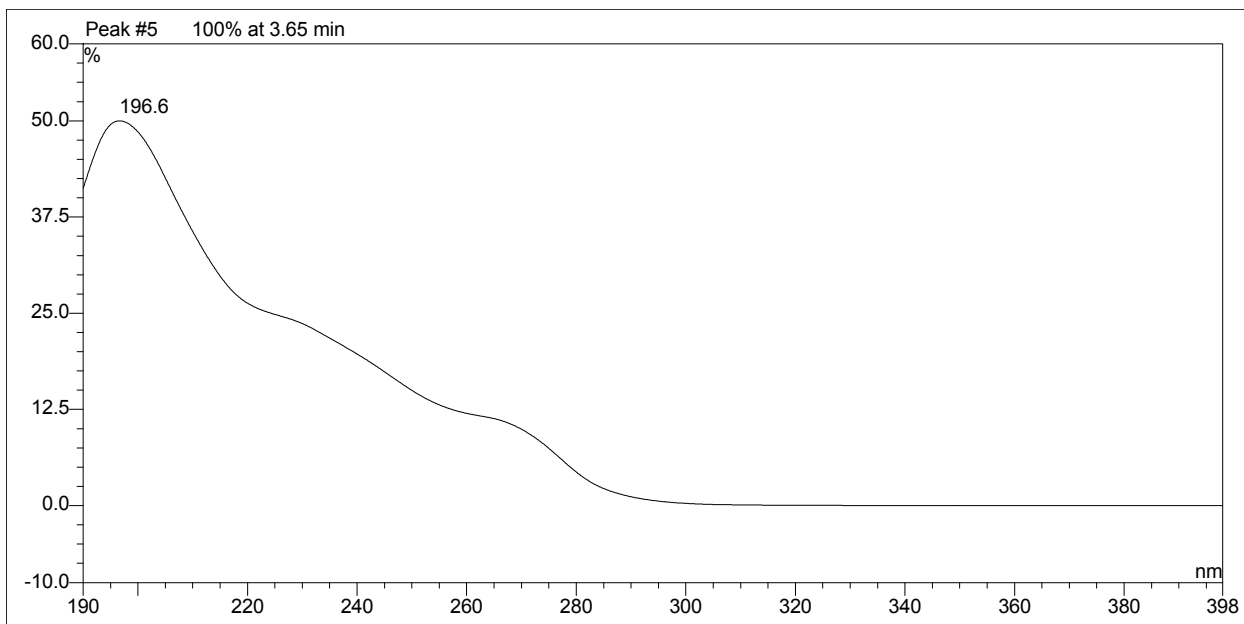
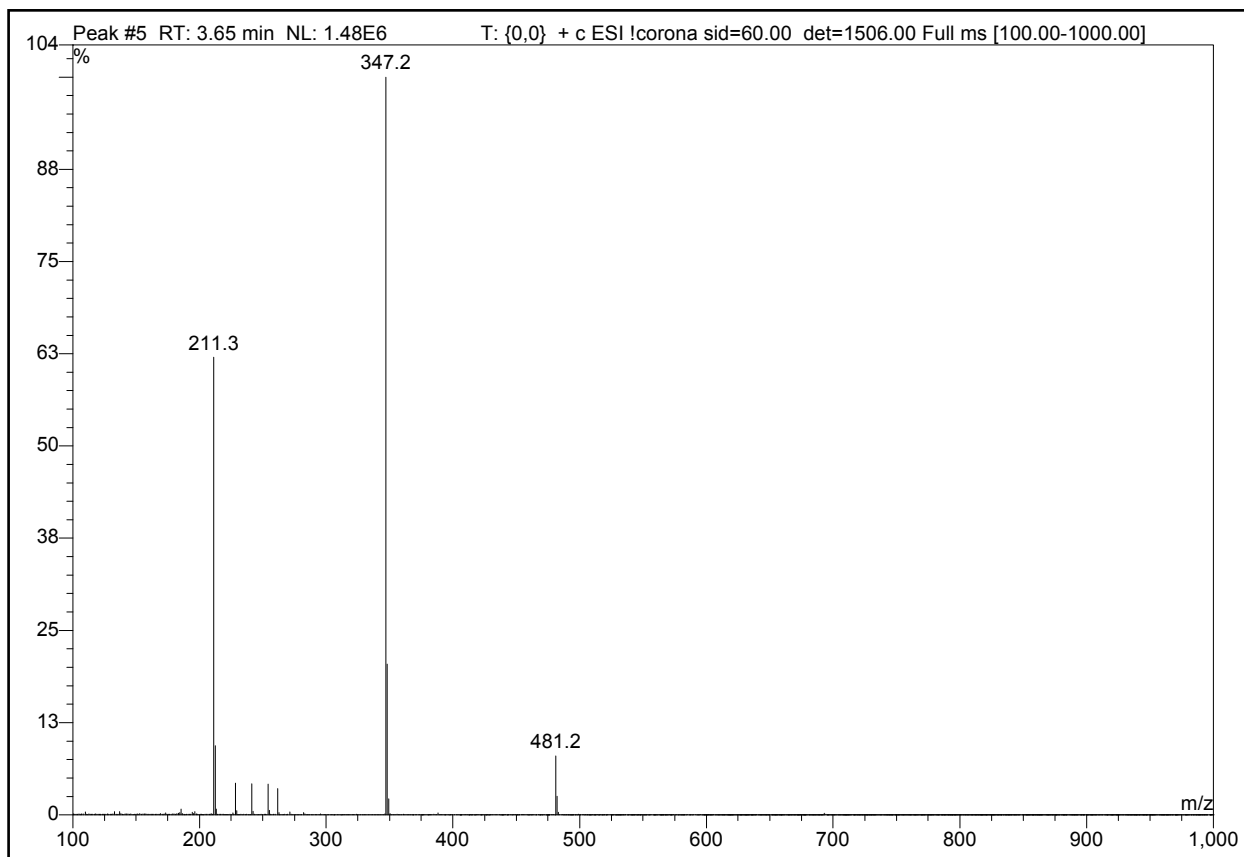
Compound 38

Sample Name: BK4309001_2 **Injection Volume:** 5.0 uL
Control Program: Purity 5 min 5-100% positive Column B **UserID** UY
Recording Time: 3/9/2016 10:42

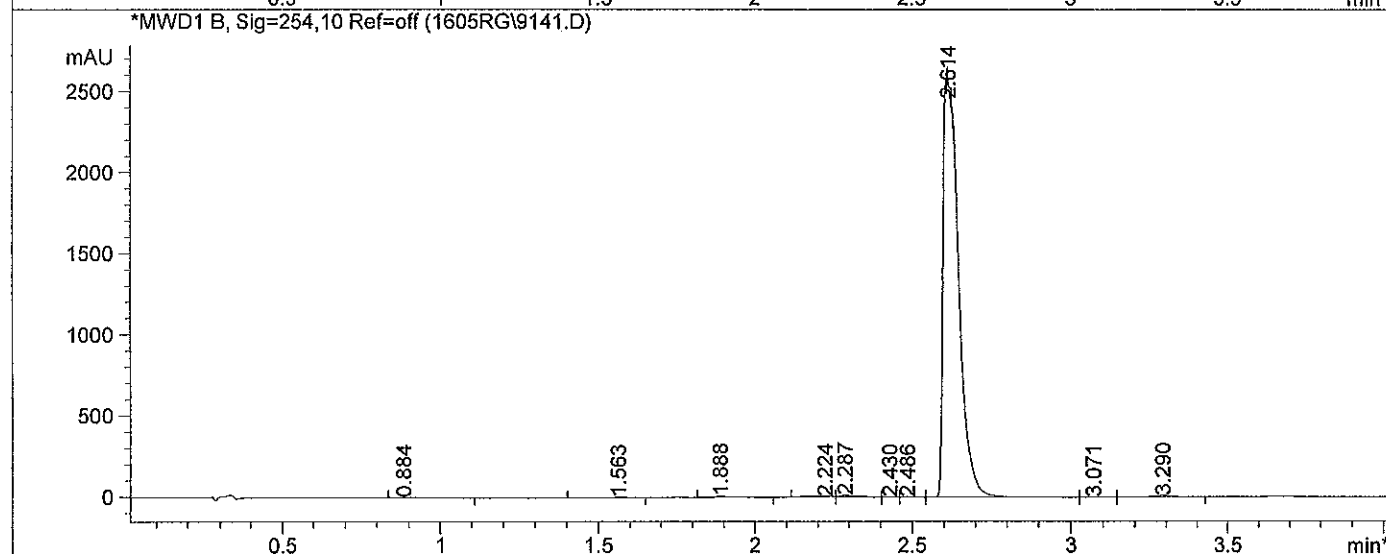
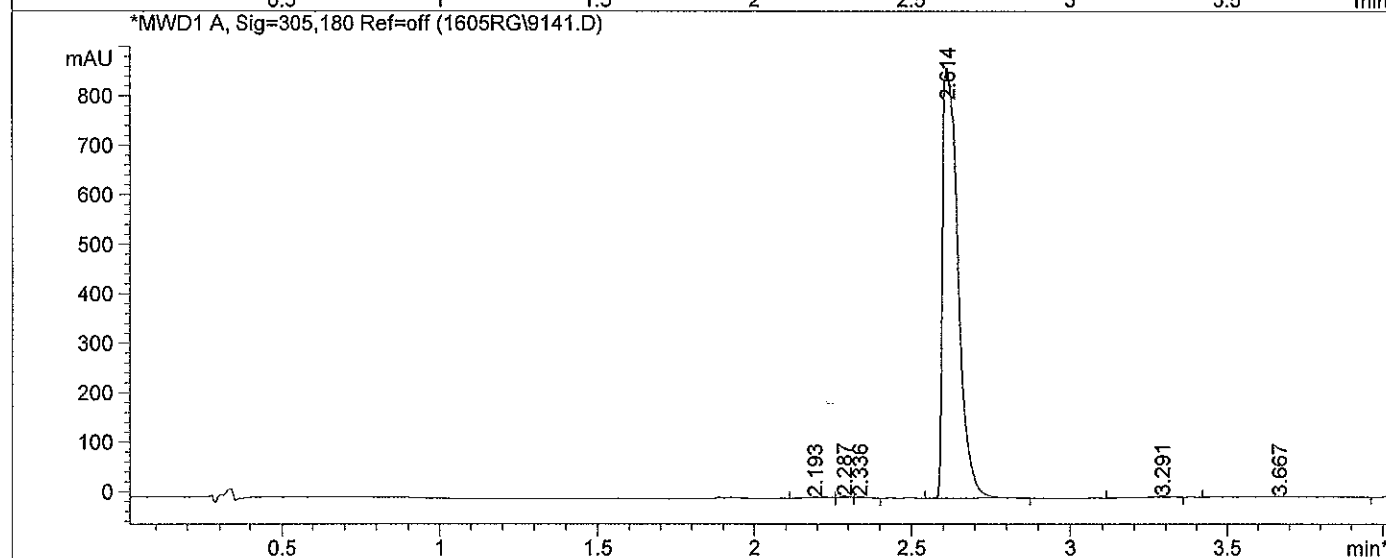
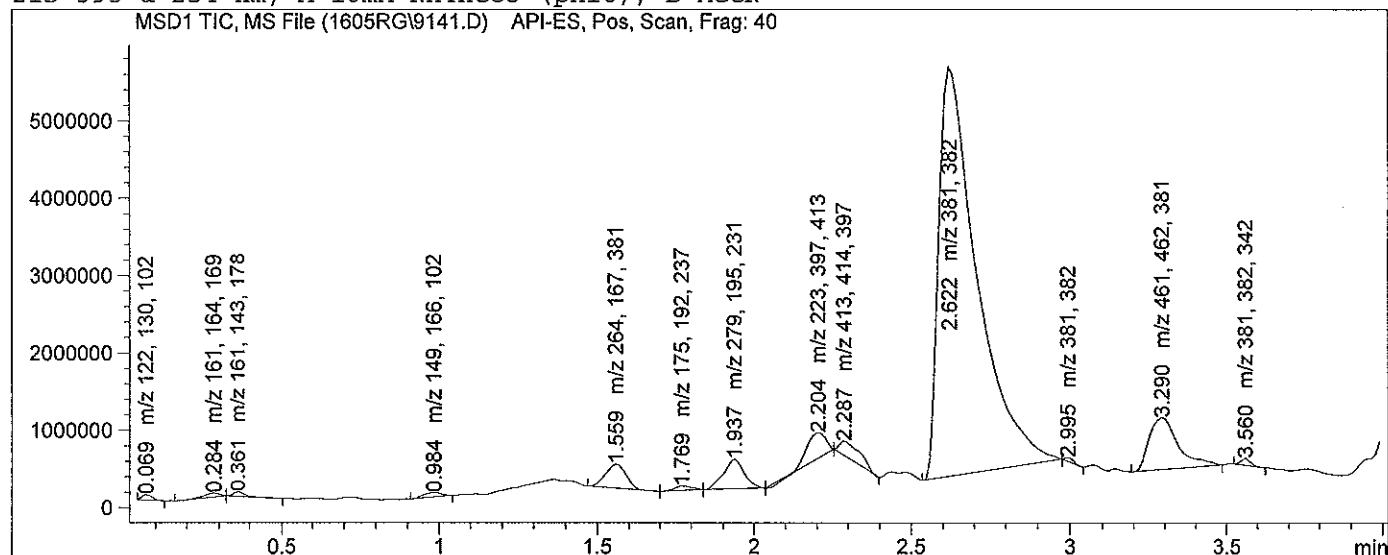
**Highest m/z responses**

No.	Ret.Time min	Height mAU	Area mAU*min	Rel.Area %	Mass - 1 m/z	Mass - 2 m/z	Mass - 3 m/z
1	0.48	20.492	1.062	6.41	141	119	115
2	1.03	3.145	0.174	1.05	137	179	162
3	2.99	2.159	0.087	0.52	227	127	196
4	3.57	0.186	0.000	0.00	347	211	348
5	3.65	370.104	15.247	92.02	347	211	348

Ignoring integration of
void,
Purity @ 254 nm=
15247/(15247+87
+174)=98%

Sample Name: BK4309001_2**Injection Volume:** 5.0 μ L**Control Program** Purity 5 min 5-100% positive Column B**UserID** UY**Recording Time:** 3/9/2016 10:42

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Injection Date : 5/25/2016 8:29:24 AM Seq. Line : 1
Sample Name : UU_BL4012001 Location : Vial 25
Acq. Operator : Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : Inj prog
Sequence File : C:\HPCHEM\1\SEQUENCE\USETHIS.S
Method : C:\HPCHEM\1\METHODS\STANDARD\SX1097X3.M
Last changed : 10/17/2013 1:29:39 PM by Doris_rg
STANDARD METHOD FOR REGISTRATION INTO CHEMSPEC
XTerra C18 50x3.0 mm, 10-97% acetonitrile in 3 min, 1 mL/min
215-395 & 254 nm, A=10mM NH4HCO3 (pH10), B=MeCN
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 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.069	BB	0.0362	1.54794e5	7.12798e4	0.2787
2	0.284	BB	0.0585	1.85756e5	5.56530e4	0.3345
3	0.361	BB	0.0406	1.60860e5	6.29138e4	0.2896
4	0.984	BB	0.0638	2.36238e5	6.00398e4	0.4253
5	1.559	BB	0.0703	1.42714e6	3.17563e5	2.5696
6	1.769	BB	0.0582	2.40265e5	5.90042e4	0.4326
7	1.937	BB	0.0690	1.82459e6	3.89188e5	3.2852
8	2.204	BB	0.0695	1.37038e6	3.33038e5	2.4674
9	2.287	BB	0.0716	9.21870e5	1.87760e5	1.6598
10	2.622	BB	0.1228	4.44370e7	5.30440e6	80.0091
11	2.995	BB	0.0291	8.54685e4	5.43063e4	0.1539
12	3.290	BB	0.0964	4.30969e6	6.71186e5	7.7596
13	3.560	BB	0.0338	1.85880e5	9.40118e4	0.3347

Totals : 5.55399e7 7.66034e6

Signal 2: MWD1 A, Sig=305,180 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.193	BB	0.0582	10.48915	2.25637	0.3478
2	2.287	BB	0.0275	5.09741	3.05635	0.1690
3	2.336	BB	0.0271	3.25371	1.99251	0.1079
4	2.614	BB	0.0543	2952.35376	853.93353	97.8915
5	3.291	BB	0.0443	10.55061	3.39270	0.3498
6	3.667	BB	0.1973	34.20100	2.10731	1.1340

Totals : 3015.94565 866.73877

Signal 3: MWD1 B, Sig=254,10 Ref=off

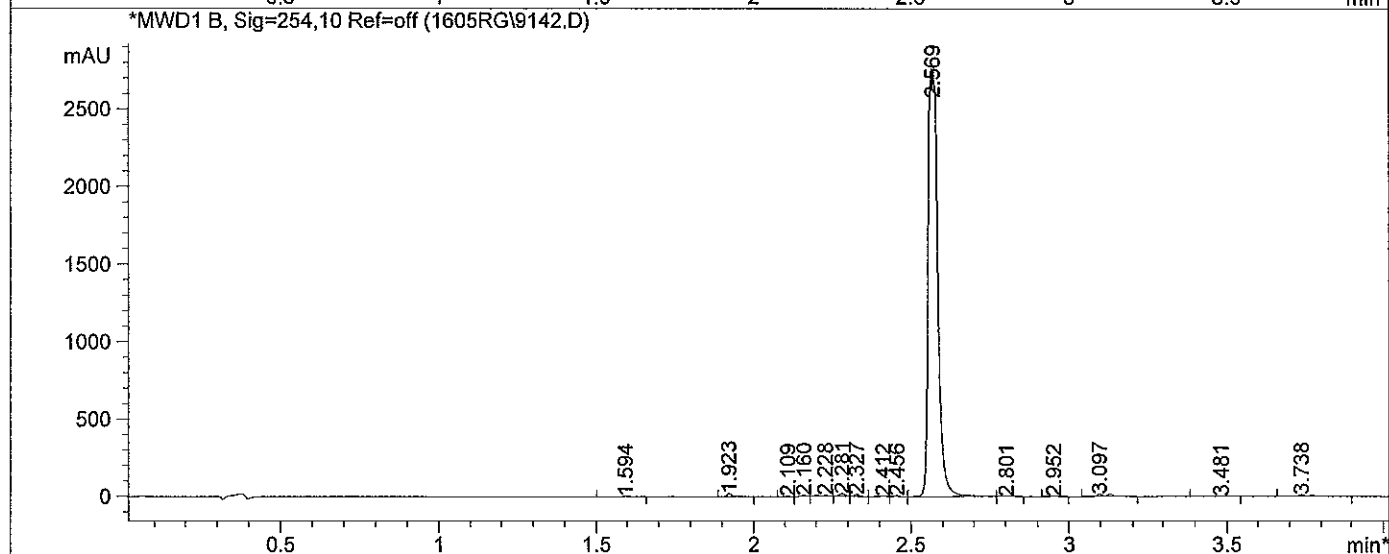
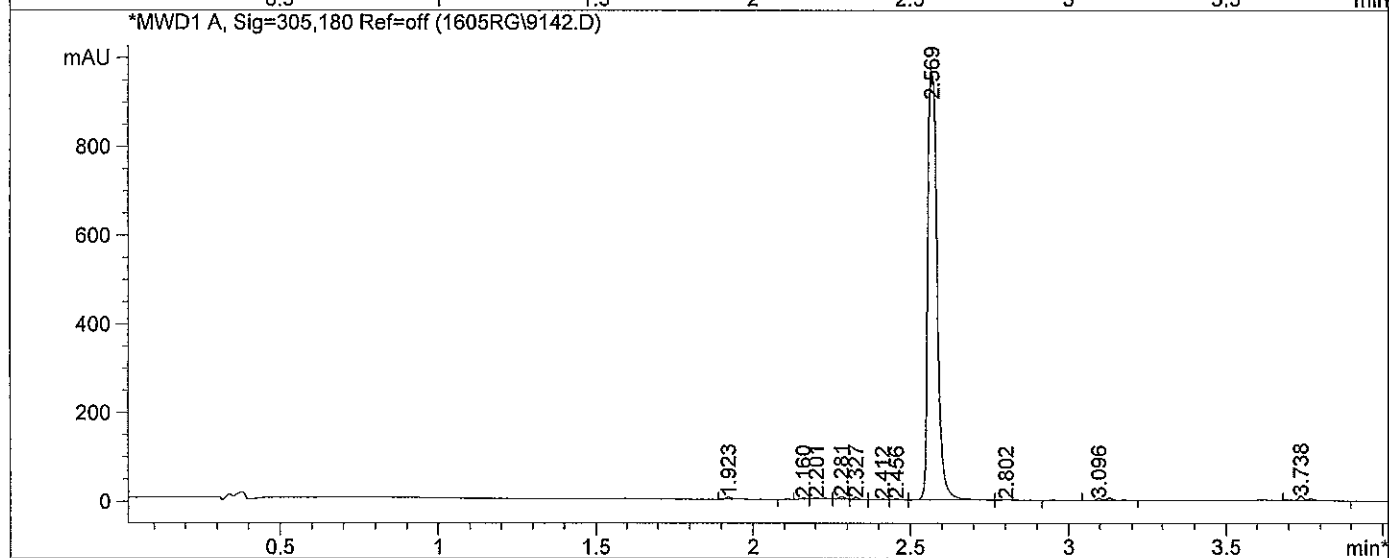
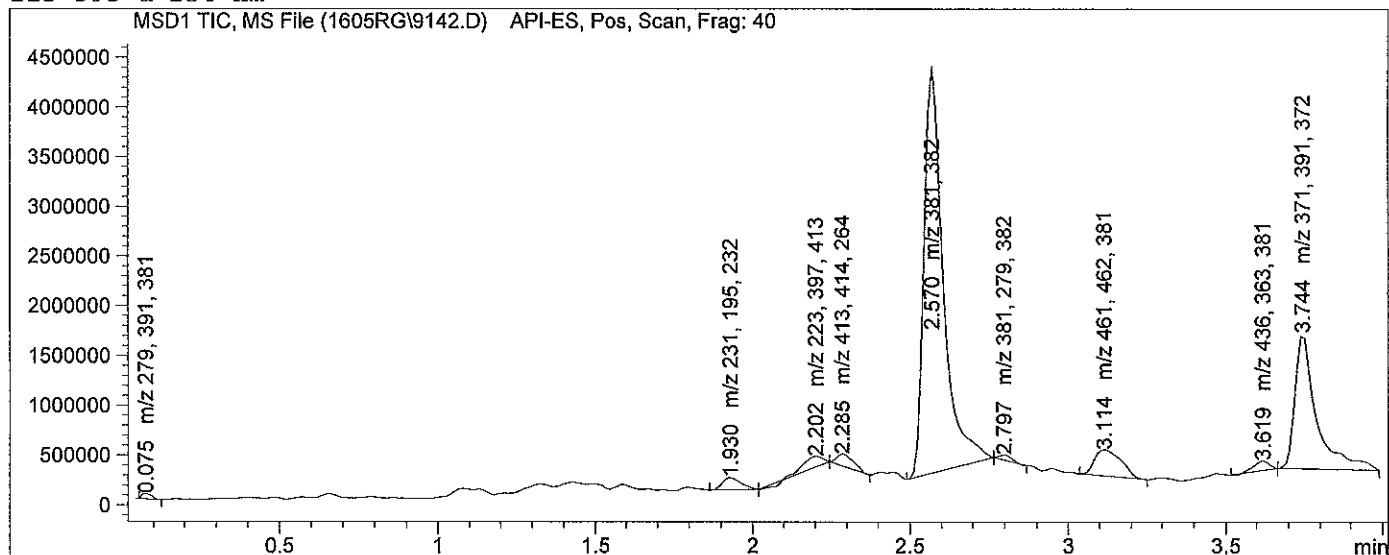
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.884	BB	0.0283	2.72638	1.73521	0.0303
2	1.563	BB	0.0445	9.33833	2.98765	0.1039
3	1.888	BB	0.0503	36.85956	10.16970	0.4100
4	2.224	BB	0.0776	27.55795	5.05657	0.3065
5	2.287	BB	0.0497	41.40025	11.58893	0.4605
6	2.430	BB	0.0243	3.97501	2.53439	0.0442
7	2.486	BB	0.0384	8.00151	3.53725	0.0890
8	2.614	BB	0.0542	8808.94336	2553.83545	97.9831
9	3.071	BB	0.0347	4.37805	1.90964	0.0487
10	3.290	BB	0.0552	47.09093	11.63870	0.5238

Totals : 8990.27134 2604.99349

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 *** End of Report ***

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Injection Date : 5/25/2016 8:35:38 AM Seq. Line : 2
Sample Name : UU_BL4012001 Location : Vial 25
Acq. Operator : Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : Inj prog
Sequence File : C:\HPCHEM\1\SEQUENCE\USETHIS.S
Method : C:\HPCHEM\1\METHODS\STANDARD\ST1097A3.M
Last changed : 10/17/2013 1:15:50 PM by Doris_rg
STANDARD METHOD FOR REGISTRATION INTO CHEMSPEC
ACE 3 C8 50x3.0 mm, 10-97% acetonitrile in 3 min, 1 ml/min
215-395 & 254 nm



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 Area Percent Report
 =====

Sorted By : Signal
 Multiplier : 1.0000
 Dilution : 1.0000
 Use Multiplier & Dilution Factor with ISTDs

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.075	BB	0.0357	1.14547e5	5.34858e4	0.4187
2	1.930	BB	0.0623	5.13503e5	1.24758e5	1.8769
3	2.202	BB	0.0717	4.31370e5	1.07799e5	1.5767
4	2.285	BB	0.0652	4.58781e5	1.22536e5	1.6769
5	2.570	BB	0.0638	1.73250e7	4.08582e6	63.3262
6	2.797	BB	0.0449	1.42587e5	5.44236e4	0.5212
7	3.114	BB	0.0869	1.57473e6	2.66068e5	5.7559
8	3.619	BB	0.0500	3.44824e5	1.02329e5	1.2604
9	3.744	BBA	0.0695	6.45302e6	1.36433e6	23.5870

Totals : 2.73584e7 6.28155e6

Signal 2: MWD1 A, Sig=305,180 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.923	BB	0.0301	11.24473	5.43838	0.5498
2	2.160	BB	0.0226	3.30321	2.64491	0.1615
3	2.201	BB	0.0265	5.64157	3.21607	0.2758
4	2.281	BB	0.0228	7.96274	5.53815	0.3893
5	2.327	BB	0.0192	5.79743	5.10707	0.2834
6	2.412	BB	0.0267	3.32308	1.87359	0.1625
7	2.456	BB	0.0197	3.45698	2.93842	0.1690
8	2.569	BB	0.0340	1961.52368	952.92517	95.8980
9	2.802	BB	0.0225	2.98798	2.11471	0.1461
10	3.096	BB	0.0425	17.16403	5.48962	0.8391
11	3.738	BB	0.0376	23.02063	10.19271	1.1255

Totals : 2045.42606 997.47880

Signal 3: MWD1 B, Sig=254,10 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.594	BB	0.0238	5.77020	3.78600	0.0966
2	1.923	BB	0.0251	34.44609	21.03387	0.5767
3	2.109	BB	0.0185	4.06588	3.78550	0.0681
4	2.160	BB	0.0229	10.20430	7.99901	0.1709
5	2.228	BB	0.0378	14.30338	7.01762	0.2395
6	2.281	BB	0.0229	25.16608	17.36719	0.4214
7	2.327	BB	0.0192	15.89354	14.01840	0.2661
8	2.412	BB	0.0269	8.35648	4.66966	0.1399
9	2.456	BB	0.0195	9.12607	7.89513	0.1528
10	2.569	BB	0.0349	5748.65088	2694.64624	96.2527
11	2.801	BB	0.0224	2.98658	2.11936	0.0500
12	2.952	BB	0.0234	4.96204	3.33090	0.0831
13	3.097	BB	0.0412	50.64235	16.79495	0.8479
14	3.481	BB	0.0440	6.06350	1.86353	0.1015
15	3.738	BB	0.0498	31.82054	10.65368	0.5328

Sample Name: B09961001

Compound 43

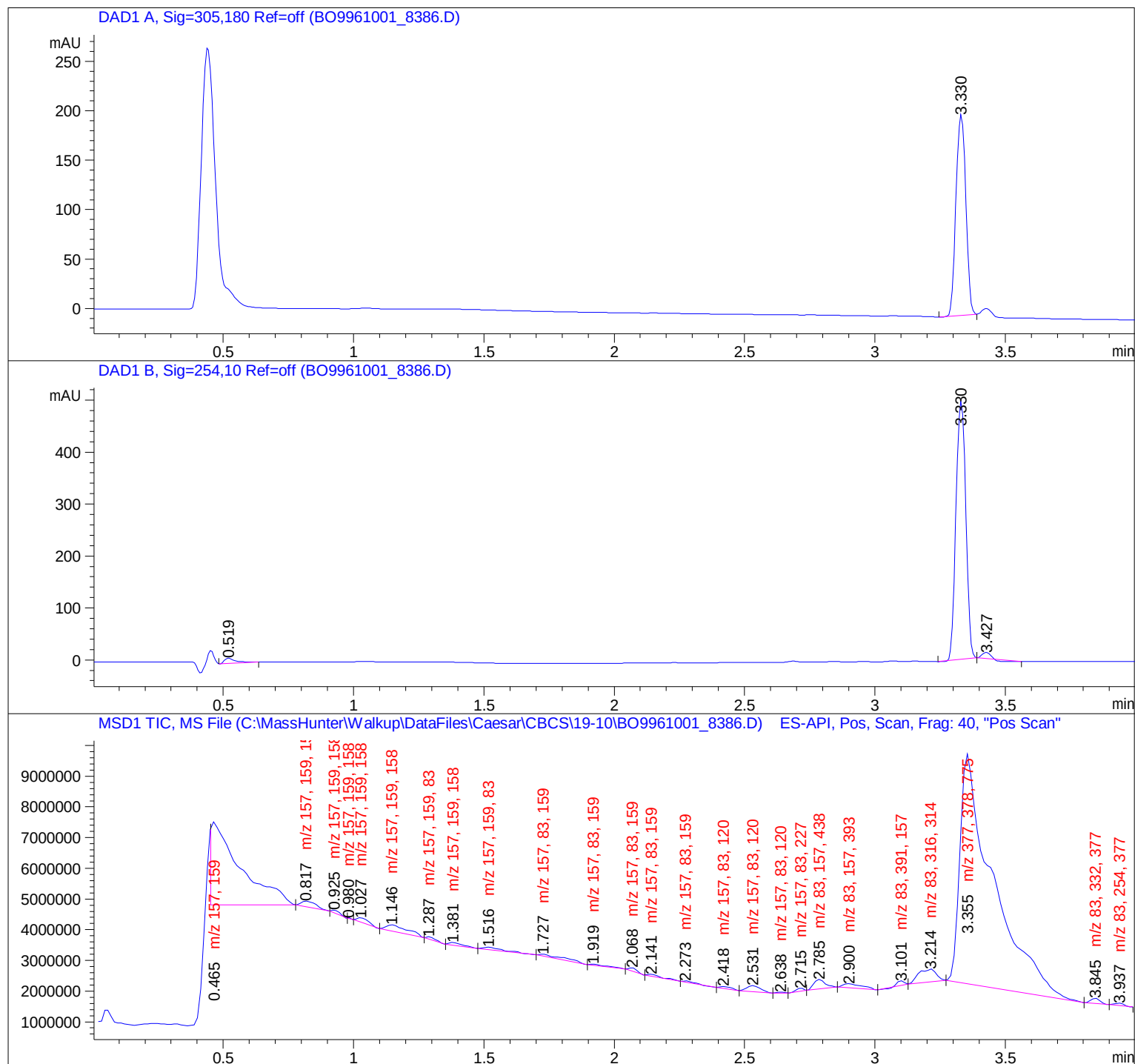
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Acq. Operator : Administrator
Sample Operator : Martin Haraldsson
Acq. Instrument : Caesar Location : D1B-E9
Injection Date : 10/24/2019 5:08:28 PM Inj : 1
Inj Volume : Inj prog

Method : C:\Users\Public\Documents\ChemStation\1\Methods\A1097-3.M
Last changed : 10/24/2019 5:06:40 PM by Administrator
(modified after loading)

Method Info : ACE C8, 50x3mm, 3µ, 10-97% MeCN, 3min; 1ml/min, A: 0.1% TFA, B:MeCN.

Sample Info : Walkup method: 'A1097-3'
Target:



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=305,180 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.330	BB	0.0446	533.30359	203.14728	100.0000

Totals : 533.30359 203.14728

Signal 2: DAD1 B, Sig=254,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.519	BB	0.0454	32.08981	10.57511	2.3772
2	3.330	BB	0.0426	1303.58960	497.16165	96.5700
3	3.427	BB	0.0262	14.21075	11.71096	1.0527

Totals : 1349.89016 519.44773

Signal 3: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.465	BB	0.1292	2.10702e7	2.71881e6	21.7367
2	0.817	BB	0.0656	7.63361e5	1.91191e5	0.7875
3	0.925	BB	0.0396	1.92206e5	8.09030e4	0.1983
4	0.980	BB	9.95e-3	1.50171e4	2.51513e4	0.0155
5	1.027	BB	0.0538	4.71714e5	1.46112e5	0.4866
6	1.146	BB	0.0798	1.21925e6	2.07977e5	1.2578
7	1.287	BB	0.0435	1.58154e5	6.06229e4	0.1632
8	1.381	BB	0.0577	3.07024e5	8.86910e4	0.3167
9	1.516	BB	0.0664	3.85976e5	8.18625e4	0.3982
10	1.727	BB	0.1239	6.27078e5	6.50329e4	0.6469
11	1.919	BB	0.0573	2.01747e5	5.12536e4	0.2081
12	2.068	BB	0.0344	2.08083e5	1.05595e5	0.2147
13	2.141	BB	0.0597	2.01025e5	5.61419e4	0.2074
14	2.273	BB	0.0351	1.02484e5	4.34893e4	0.1057
15	2.418	BB	0.0525	1.74920e5	5.55030e4	0.1805
16	2.531	BB	0.0569	6.69689e5	1.87643e5	0.6909
17	2.638	BB	0.0299	5.24778e4	2.92591e4	0.0541
18	2.715	BB	0.0345	1.70901e5	9.07612e4	0.1763

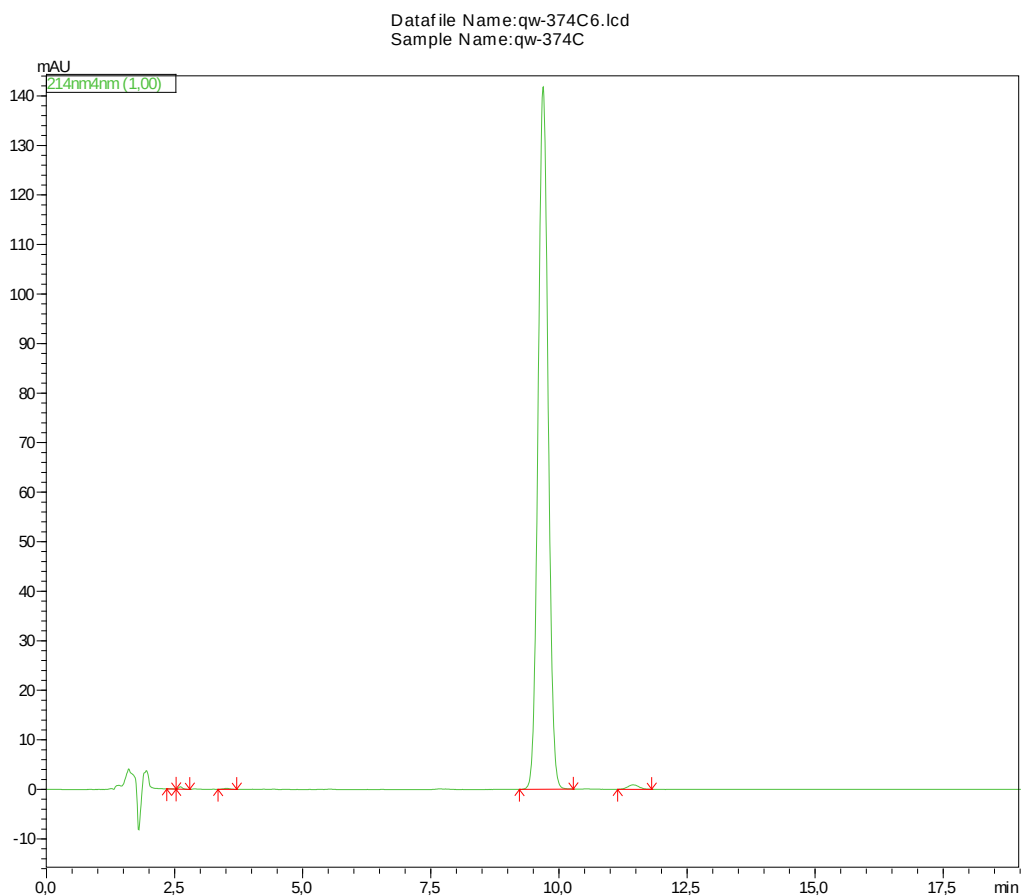
Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
19	2.785	BB	0.0457	9.32530e5	3.17607e5	0.9620
20	2.900	BB	0.0734	7.15206e5	1.34636e5	0.7378
21	3.101	BB	0.0300	2.42075e5	1.54709e5	0.2497
22	3.214	BB	0.0778	2.01969e6	4.28390e5	2.0836
23	3.355	BB	0.1172	6.54187e7	7.48085e6	67.4881
24	3.845	BB	0.0408	4.18925e5	1.66301e5	0.4322
25	3.937	BBA	0.0390	1.95232e5	8.26398e4	0.2014

Totals : 9.69337e7 1.30511e7

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*** End of Report ***

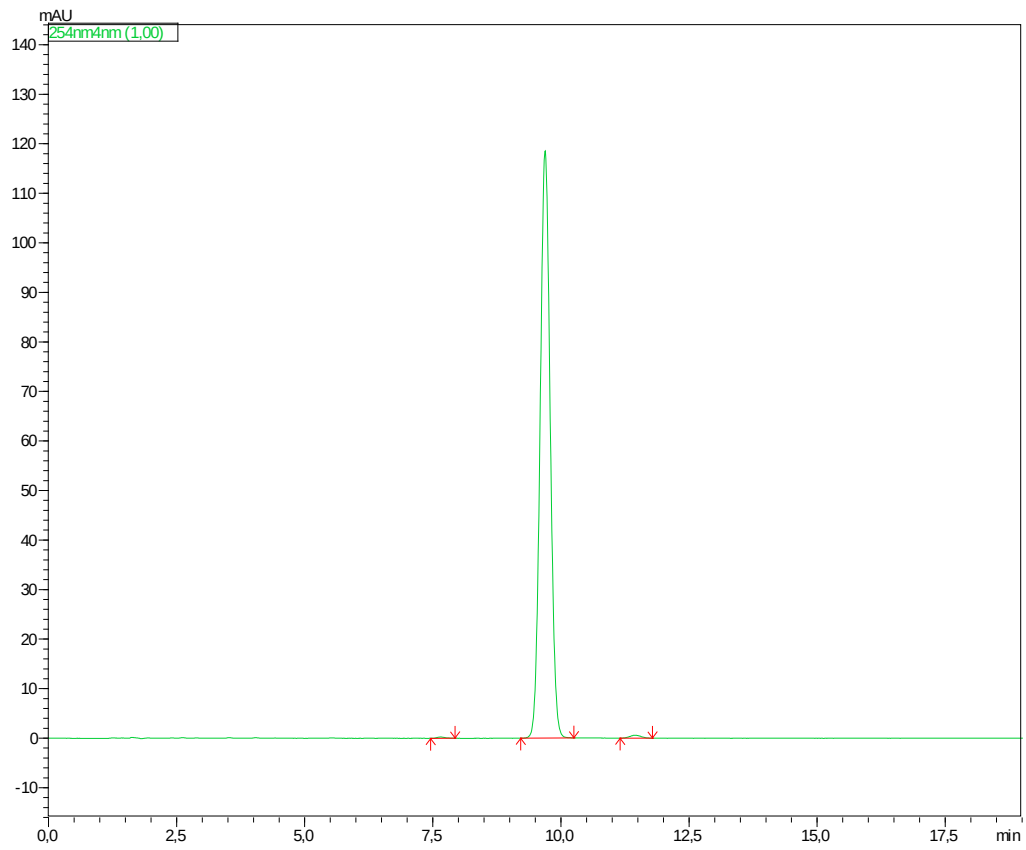
Compound 44 Analysis Report

Sample was dissolved in methanol to make ~ 0.2 mg/ml solution. Quantitative analysis was performed using NUCLEODUR C-18, HTEC, 5µm column on a SHIMADZU LC-30AD system with an Acetonitrile/water =60:40 eluent with 0.005% formic acid and a flow rate of 1.0 mL/min, SPD-M20A detector at 214 and 254 nm. Software is Labsolutions Version 5.51.



Peak#	Ret. Time	Area	Height	Conc.	Name	Area%
1	2,475	183	57	0,000		0,009
2	2,610	2570	489	0,000		0,131
3	3,517	1982	211	0,000		0,101
4	9,691	1938849	141795	0,000		99,047
5	11,447	13929	894	0,000		0,712
Total		1957514	143444	0,000		100,000

Datafile Name:qw-374C6.lcd
Sample Name:qw-374C

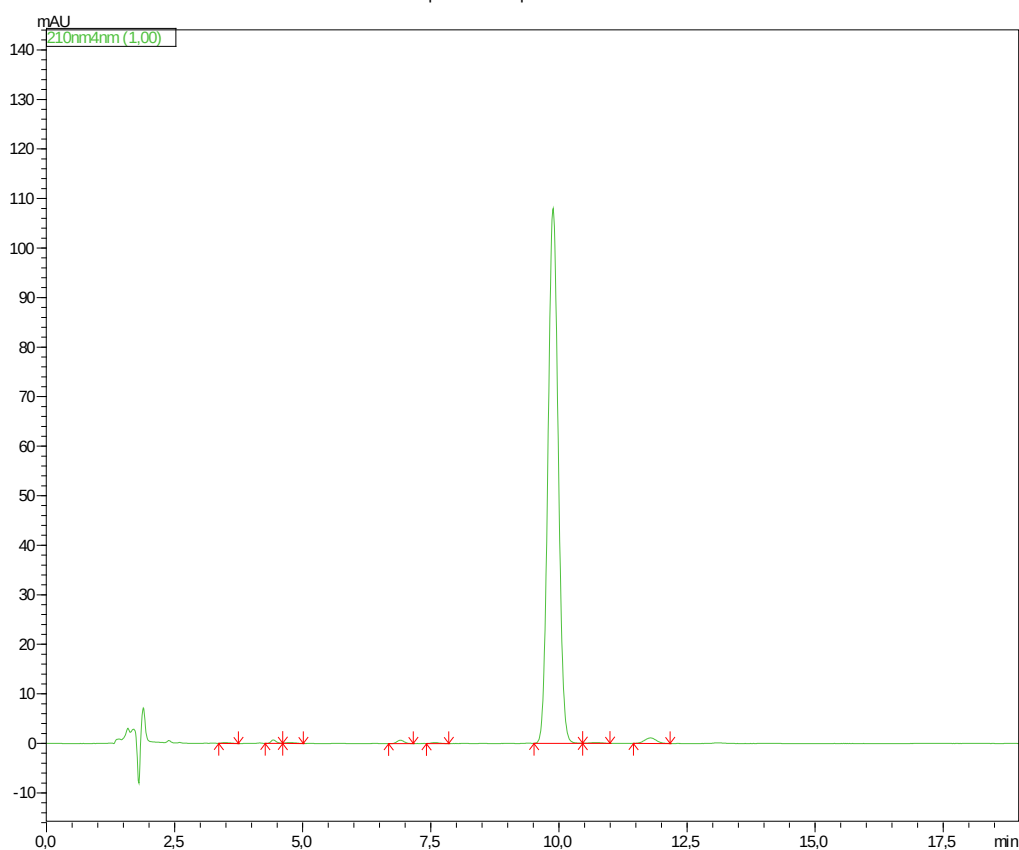


Peak#	Ret. Time	Area	Height	Conc.	Name	Area%
1	7,646	2911	250	0,000		0,179
2	9,691	1617863	118538	0,000		99,255
3	11,449	9238	595	0,000		0,567
Total		1630011	119383	0,000		100,000

Compound 45, Analysis Report

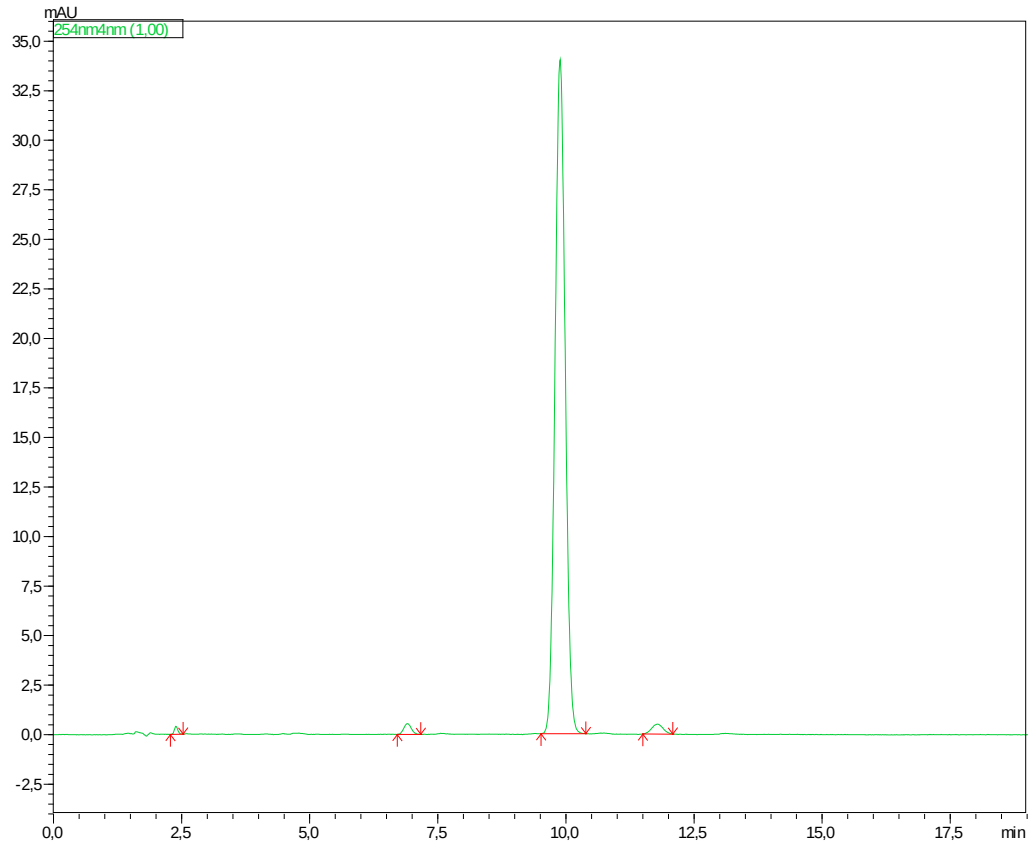
Sample was dissolved in methanol to make ~ 0.2 mg/ml solution. Quantitative analysis was performed using NUCLEODUR C-18, HTEC, 5µm column on a SHIMADZU LC-30AD system with an Acetonitrile/water =60:40 eluent with 0.005% formic acid and a flow rate of 1.0 mL/min, SPD-M20A detector at 214 and 254 nm. Software is Labsolutions Version 5.51.

Datafile Name:qw-377C3.lcd
Sample Name:qw-377C



Peak#	Ret. Time	Area	Height	Conc.	Name	Area%
1	3,479	1742	136	0,000		0,113
2	4,427	5350	700	0,000		0,348
3	4,790	2428	163	0,000		0,158
4	6,904	6844	681	0,000		0,446
5	7,591	2155	199	0,000		0,140
6	9,885	1497099	107944	0,000		97,448
7	10,731	2687	159	0,000		0,175
8	11,784	18004	1117	0,000		1,172
Total		1536310	111098	0,000		100,000

Datafile Name:qw-377C3.lcd
Sample Name:qw-377C

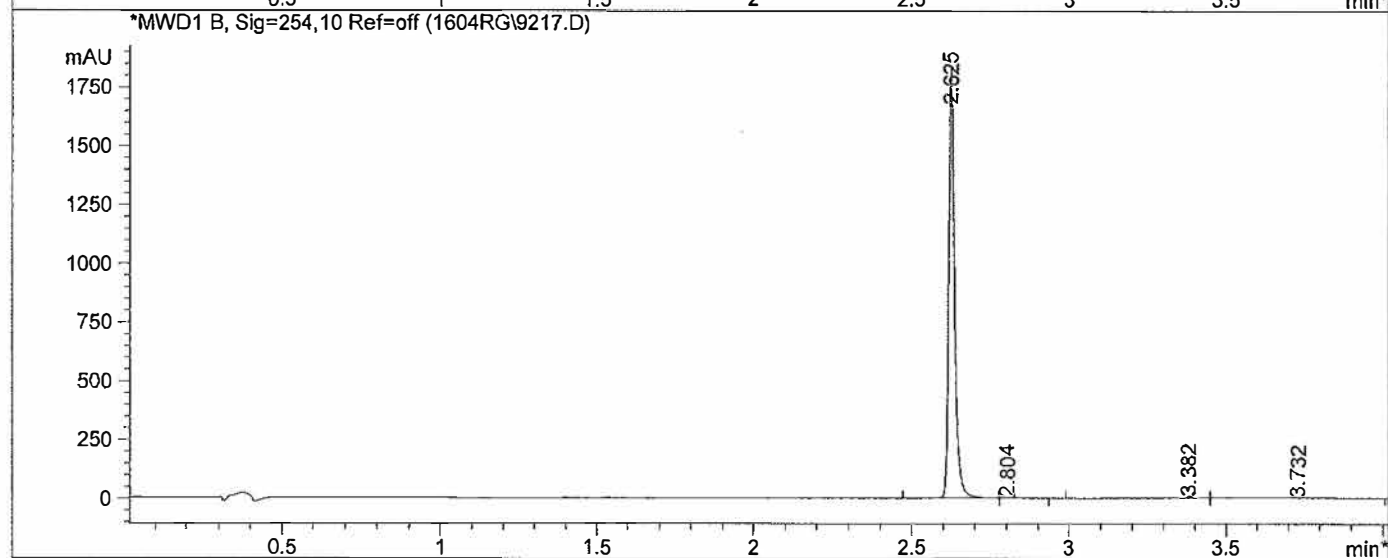
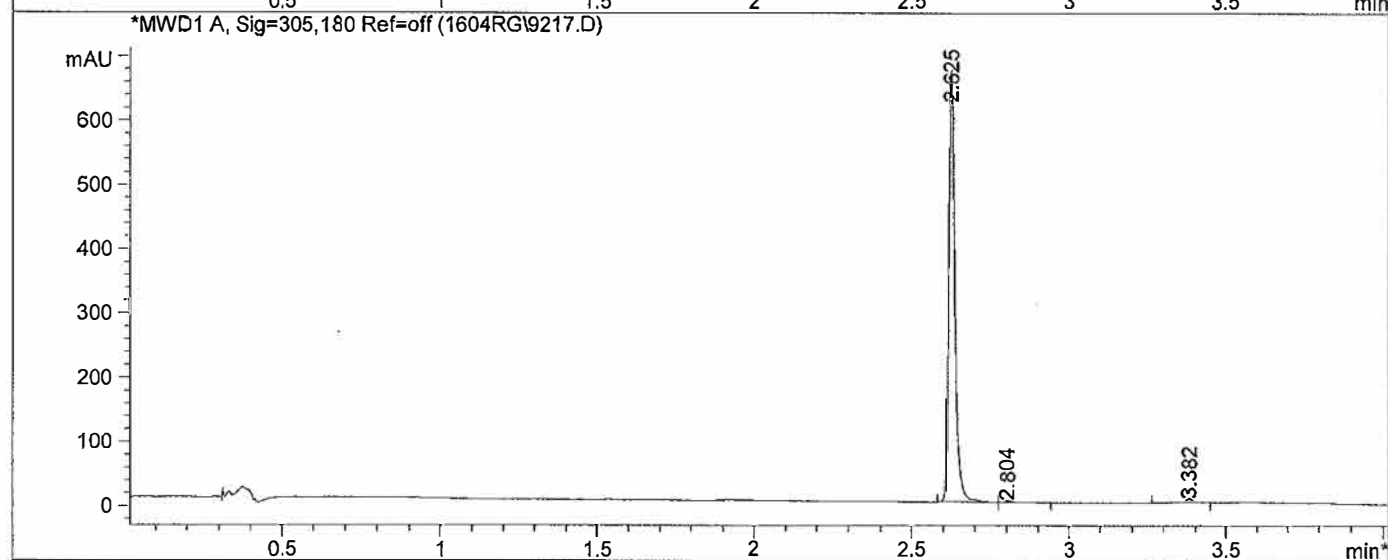
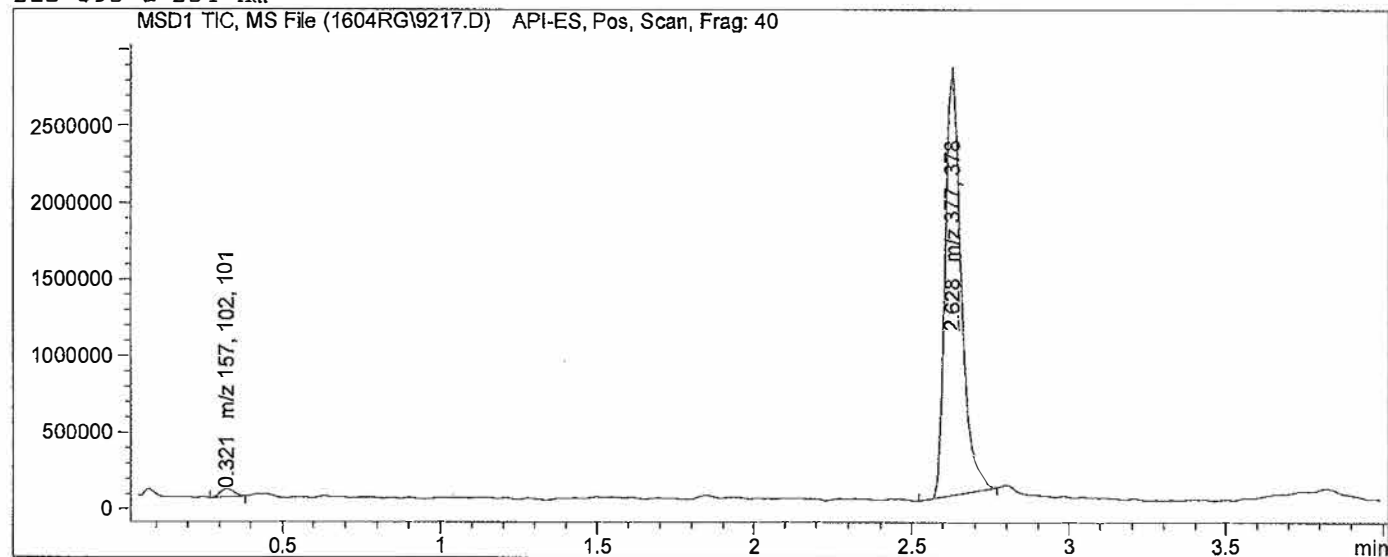


Peak#	Ret. Time	Area	Height	Conc.	Name	Area%
1	2,389	1893	404	0,000		0,389
2	6,907	5636	545	0,000		1,159
3	9,885	470847	34017	0,000		96,847
4	11,778	7799	500	0,000		1,604
Total		486175	35467	0,000		100,000

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Injection Date	: 4/25/2016 12:51:05 PM	Seq. Line	: 2
Sample Name	: BK9484 Final	Location	: Vial 1
Acq. Operator	:	Inj	: 1
Acq. Instrument	: Instrument 1	Inj Volume	: Inj prog
Sequence File	: C:\HPCHEM\1\SEQUENCE\USETHIS.S		
Method	: C:\HPCHEM\1\METHODS\STANDARD\ST1097A3.M		
Last changed	: 10/17/2013 1:15:50 PM by Doris_rg		
STANDARD METHOD FOR REGISTRATION INTO CHEMSPEC			
ACE 3 C8 50x3.0 mm, 10-97% acetonitrile in 3 min, 1 ml/min			
215-395 & 254 nm			

=====



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.321	BB	0.0485	1.61419e5	5.50541e4	1.6292
2	2.628	BB	0.0548	9.74653e6	2.80615e6	98.3708

Totals : 9.90795e6 2.86120e6

Signal 2: MWD1 A, Sig=305,180 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.625	BB	0.0227	903.21808	630.52081	98.6454
2	2.804	BBA	0.0214	3.61789	2.74093	0.3951
3	3.382	PBA	0.0230	8.78502	6.02301	0.9595

Totals : 915.62099 639.28475

Signal 3: MWD1 B, Sig=254,10 Ref=off

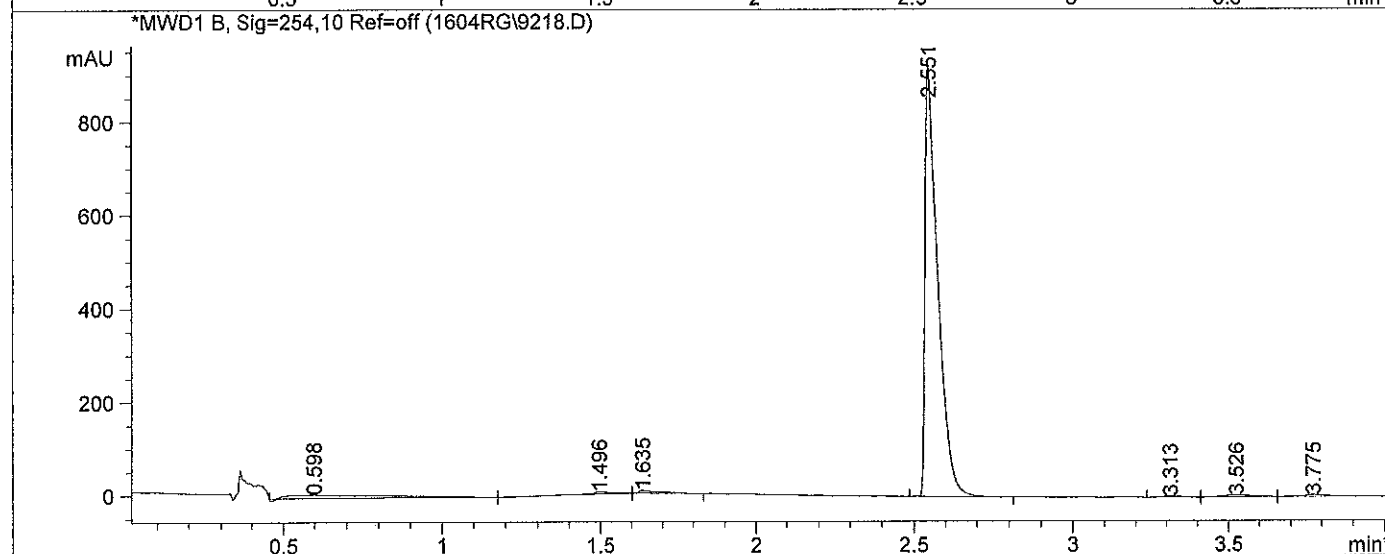
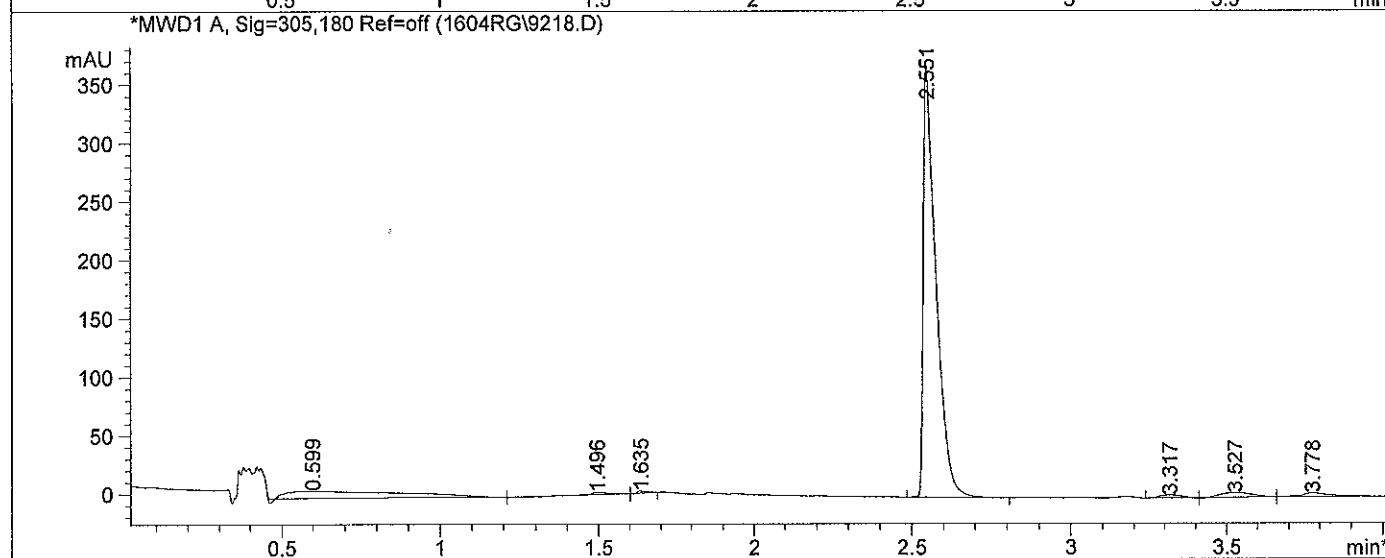
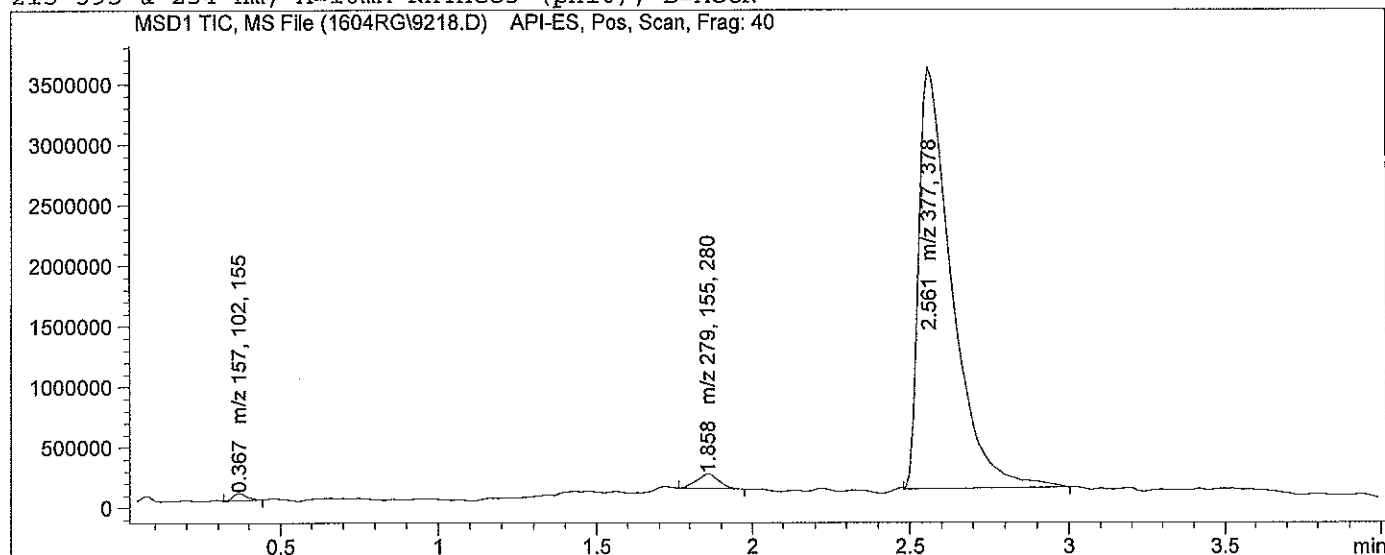
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.625	BB	0.0222	2336.28662	1677.70715	98.1932
2	2.804	BB	0.0205	3.43584	2.75675	0.1444
3	3.382	BB	0.0153	7.28600	9.16373	0.3062
4	3.732	BPA	0.2185	32.26600	1.75471	1.3561

Totals : 2379.27445 1691.38235

=====
*** End of Report ***

=====
Injection Date : 4/25/2016 12:57:22 PM Seq. Line : 3
Sample Name : BK9484 Final Location : Vial 1
Acq. Operator : Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : Inj prog
Sequence File : C:\HPCHEM\1\SEQUENCE\USETHIS.S
Method : C:\HPCHEM\1\METHODS\STANDARD\SX1097X3.M
Last changed : 10/17/2013 1:29:39 PM by Doris_rg
STANDARD METHOD FOR REGISTRATION INTO CHEMSPEC
XTerra C18 50x3.0 mm, 10-97% acetonitrile in 3 min, 1 ml/min
215-395 & 254 nm, A=10mM NH4HCO3 (pH10), B=MeCN
=====



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.367	BB	0.0478	2.02563e5	6.38124e4	0.7742
2	1.858	BB	0.0673	6.01218e5	1.23922e5	2.2978
3	2.561	BB	0.1097	2.53613e7	3.49369e6	96.9280

Totals : 2.61651e7 3.68143e6

Signal 2: MWD1 A, Sig=305,180 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.599	BB	0.3056	169.28957	6.54873	13.1131
2	1.496	BB	0.0664	10.24484	2.19635	0.7936
3	1.635	BB	0.0326	4.20271	1.99673	0.3255
4	2.551	BB	0.0410	1040.97339	367.79208	80.6334
5	3.317	BB	0.0827	14.32223	2.75153	1.1094
6	3.527	BB	0.1273	31.29874	4.18440	2.4244
7	3.778	BBA	0.0922	20.66326	3.16335	1.6006

Totals : 1290.99473 388.63317

Signal 3: MWD1 B, Sig=254,10 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.598	BB	0.2770	185.72829	8.05617	6.3375
2	1.496	BB	0.0821	30.60085	5.09364	1.0442
3	1.635	BB	0.0700	33.74491	6.34506	1.1515
4	2.551	BB	0.0409	2607.42114	924.44348	88.9722
5	3.313	BB	0.0809	13.72308	2.71680	0.4683
6	3.526	BB	0.1251	31.38525	4.20279	1.0709
7	3.775	BBA	0.0881	27.99907	4.40612	0.9554

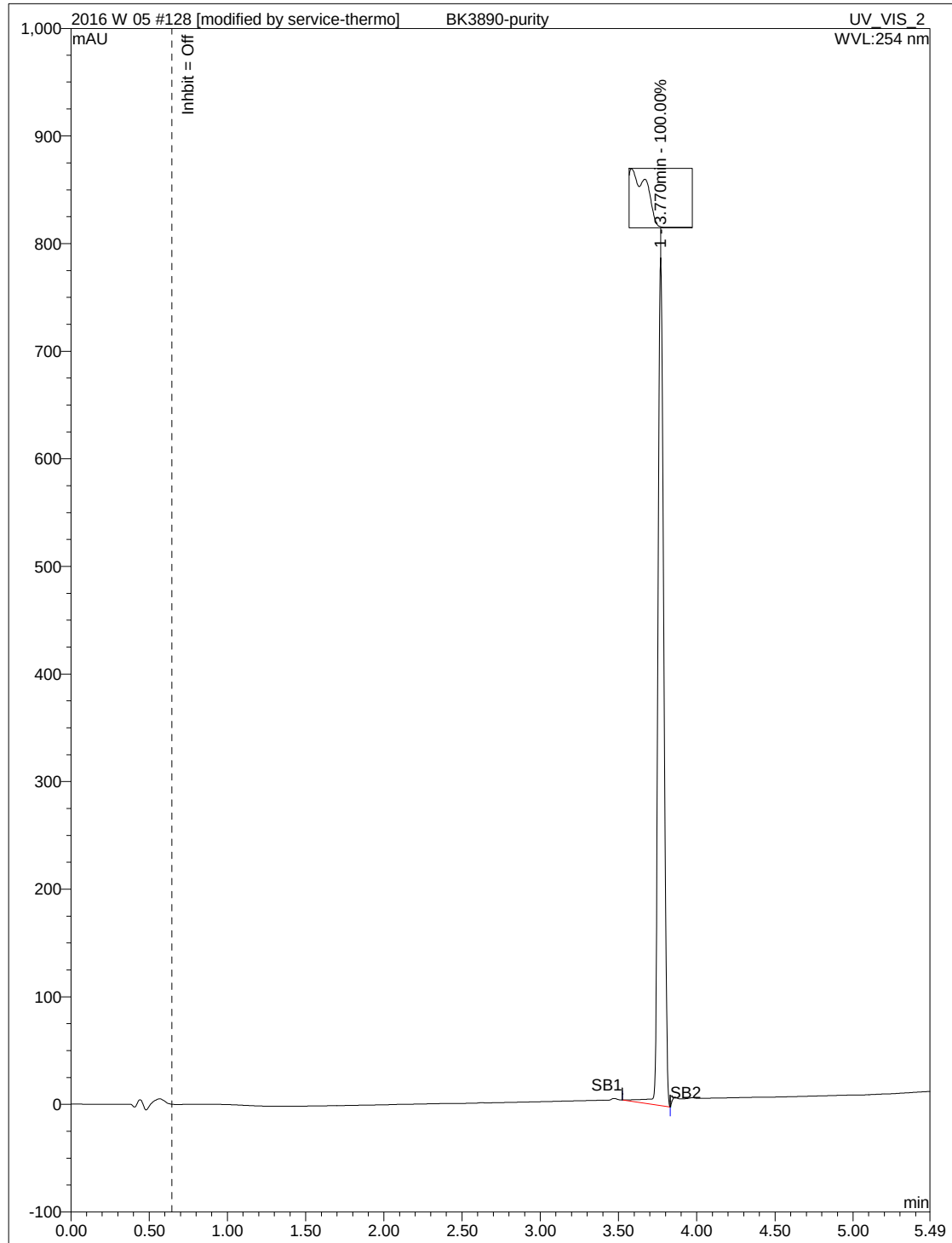
Totals : 2930.60260 955.26406

=====
*** End of Report ***
=====

Compound 47

Sample Name: BK3890-purity
Control Program: Purity 5 min 5-100% positive Column B
Recording Time: 2/2/2016 14:47

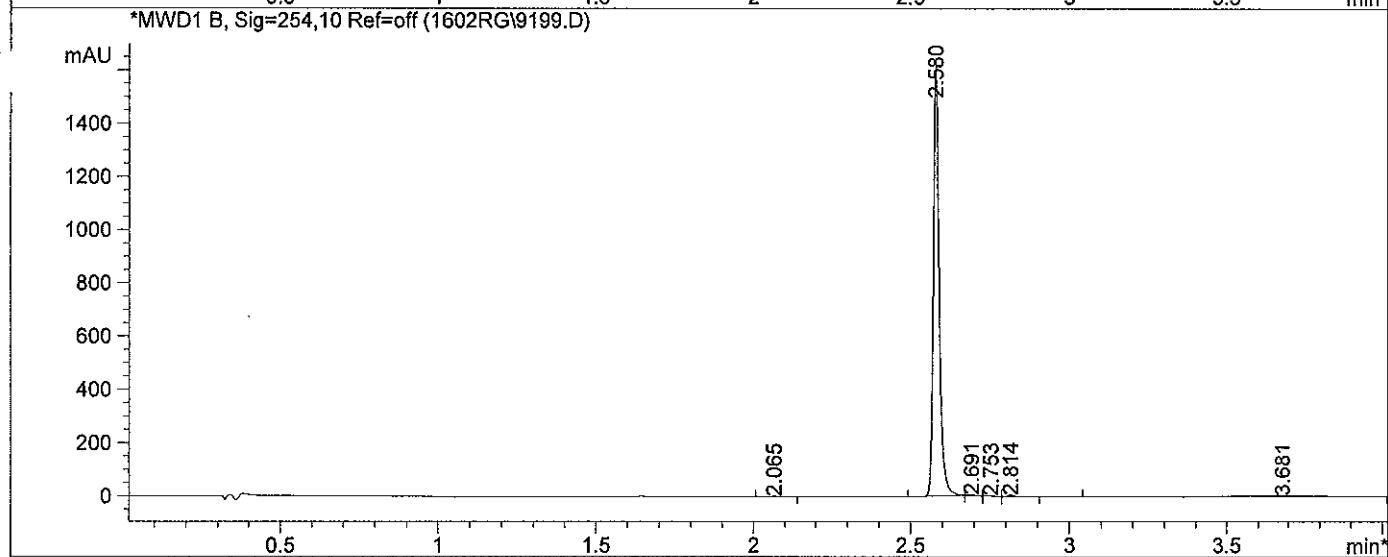
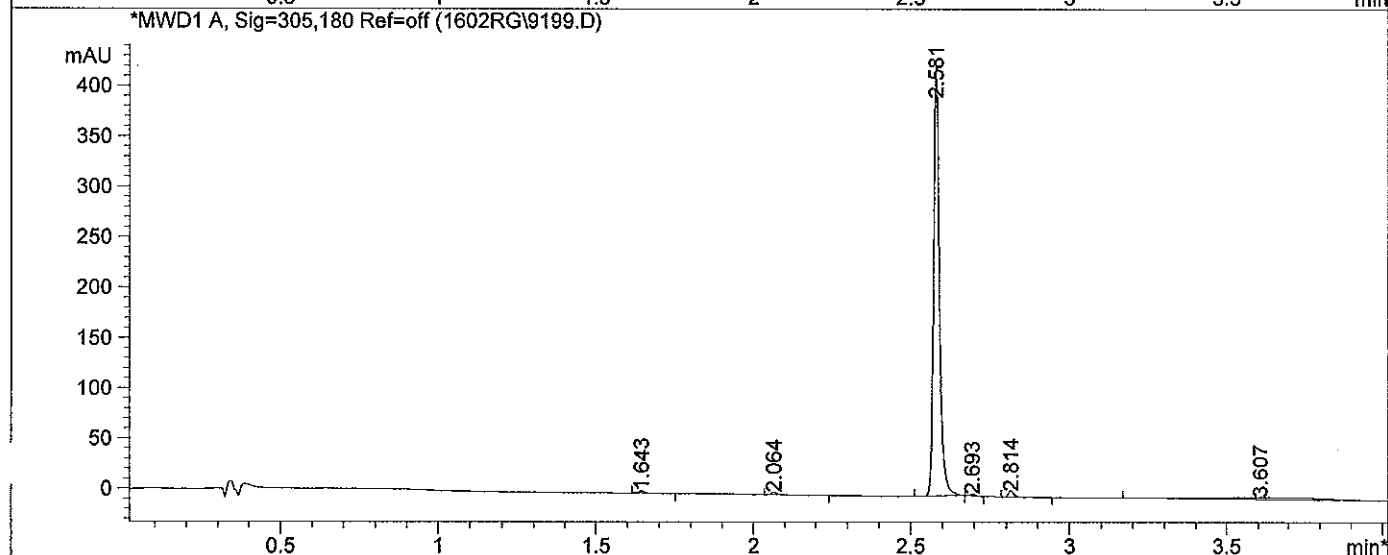
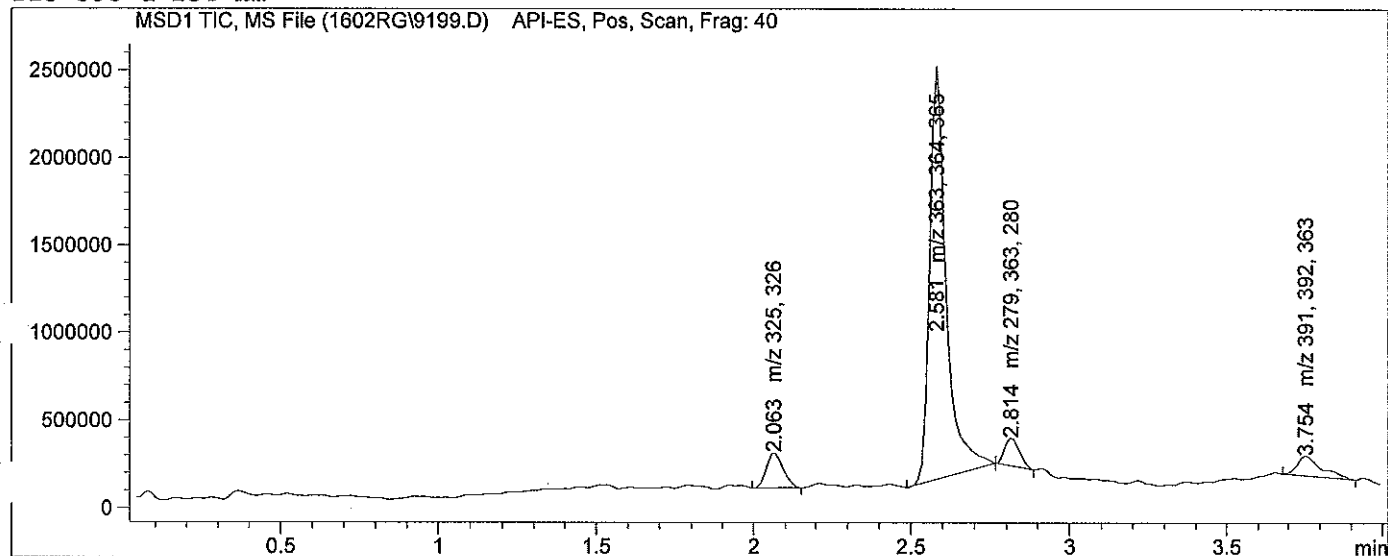
Injection Volume: 1.0 μ L
UserID: Neeraj G



Highest m/z responses

No.	Ret.Time min	Height mAU	Area mAU*min	Rel.Area %	Mass - 1 m/z	Mass - 2 m/z	Mass - 3 m/z
1	3.77	788.183	32.921	100.00	377	378	211

=====
Injection Date : 2/22/2016 10:30:06 AM Seq. Line : 1
Sample Name : BS7745001 Location : Vial 5
Acq. Operator : Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : Inj prog
Sequence File : C:\HPCHEM\1\SEQUENCE\USETHIS.S
Method : C:\HPCHEM\1\METHODS\STANDARD\ST1097A3.M
Last changed : 10/17/2013 1:15:50 PM by Doris_rg
STANDARD METHOD FOR REGISTRATION INTO CHEMSPEC
ACE 3 C8 50x3.0 mm, 10-97% acetonitrile in 3 min, 1 ml/min
215-395 & 254 nm



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Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	2.063	BB	0.0562	7.32424e5	2.04169e5	7.0465
2	2.581	BB	0.0530	8.53962e6	2.35725e6	82.1580
3	2.814	BB	0.0521	5.15423e5	1.59306e5	4.9588
4	3.754	BB	0.0767	6.06670e5	1.13412e5	5.8367

Totals : 1.03941e7 2.83414e6

Signal 2: MWD1 A, Sig=305,180 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	1.643	BBA	0.0216	3.21073	2.39745	0.5167
2	2.064	PBA	0.0208	3.19829	2.52624	0.5147
3	2.581	BB	0.0218	547.92712	404.96161	88.1727
4	2.693	BB	0.0190	1.98062	1.78415	0.3187
5	2.814	BB	0.0217	8.22169	6.09889	1.3230
6	3.607	BBA	0.3456	56.88654	1.97779	9.1542

Totals : 621.42498 419.74613

Signal 3: MWD1 B, Sig=254,10 Ref=off

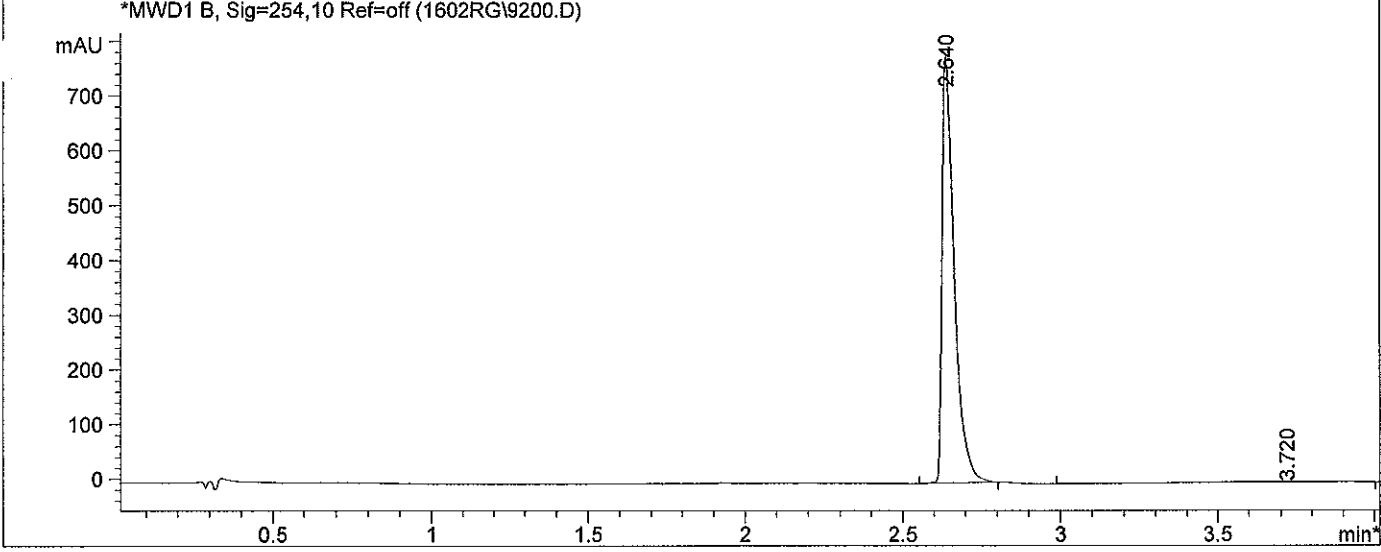
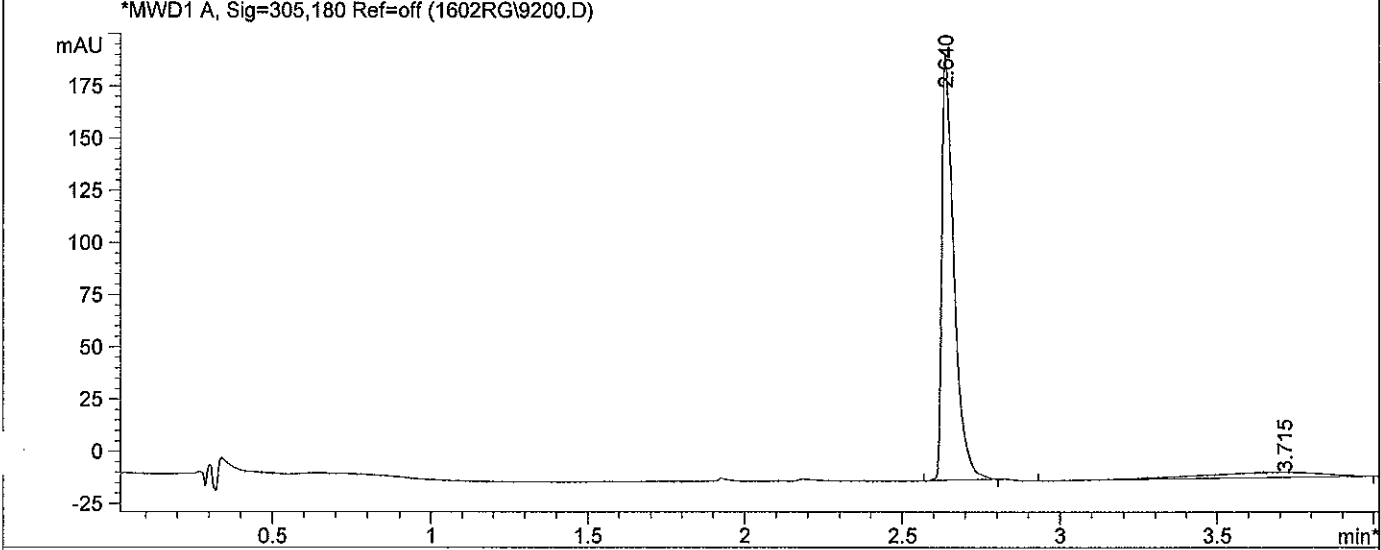
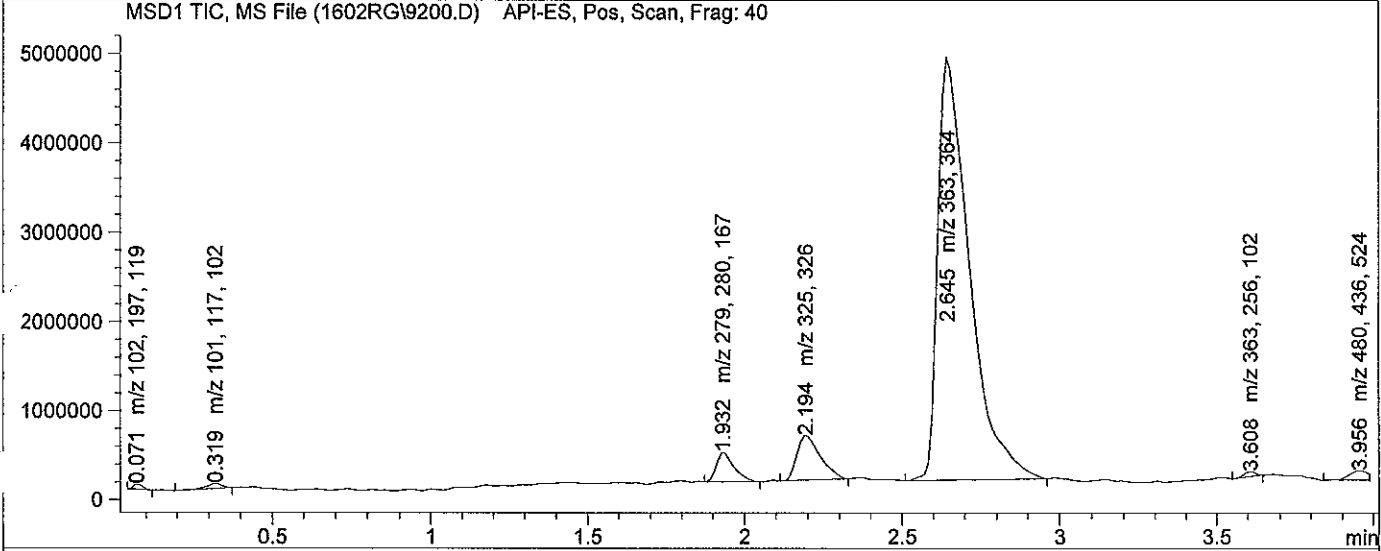
Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.065	BB	0.0261	3.10030	1.79761	0.1418
2	2.580	BB	0.0218	2086.33423	1536.74414	95.4309
3	2.691	BB	0.0212	4.19295	3.29950	0.1918
4	2.753	BB	0.0207	4.07651	3.24015	0.1865
5	2.814	BB	0.0219	8.52774	6.25697	0.3901
6	3.681	BBA	0.3317	79.99281	2.86522	3.6589

Totals : 2186.22454 1554.20359

=====
*** End of Report ***

=====
Injection Date : 2/22/2016 10:36:22 AM Seq. Line : 2
Sample Name : BS7745001 Location : Vial 5
Acq. Operator : Inj : 1
Acq. Instrument : Instrument 1 Inj Volume : Inj prog
Sequence File : C:\HPCHEM\1\SEQUENCE\USETHIS.S
Method : C:\HPCHEM\1\METHODS\STANDARD\SX1097X3.M
Last changed : 10/17/2013 1:29:39 PM by Doris_rg
STANDARD METHOD FOR REGISTRATION INTO CHEMSPEC
XTerra C18 50x3.0 mm, 10-97% acetonitrile in 3 min, 1 ml/min
215-395 & 254 nm, A=10mM NH4HCO3 (pH10), B=MeCN



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Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: MSD1 TIC, MS File

Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.071	BB	0.0313	1.16718e5	6.20658e4	0.3077
2	0.319	BB	0.0509	2.07884e5	6.03618e4	0.5480
3	1.932	BB	0.0598	1.31026e6	3.36011e5	3.4538
4	2.194	BB	0.0814	2.60112e6	5.06400e5	6.8565
5	2.645	BB	0.1098	3.30906e7	4.75498e6	87.2263
6	3.608	BB	0.0458	1.60347e5	5.93906e4	0.4227
7	3.956	BBA	0.0686	4.49560e5	1.09159e5	1.1850

Totals : 3.79364e7 5.88837e6

Signal 2: MWD1 A, Sig=305,180 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.640	PB	0.0447	548.96899	195.73953	88.4346
2	3.715	BBA	0.3460	71.79393	2.52276	11.5654

Totals : 620.76292 198.26229

Signal 3: MWD1 B, Sig=254,10 Ref=off

Signal has been modified after loading from rawdata file!

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.640	BB	0.0447	2111.32080	754.33685	97.2023
2	3.720	PB	0.2888	60.76918	2.48949	2.7977

Totals : 2172.08998 756.82634

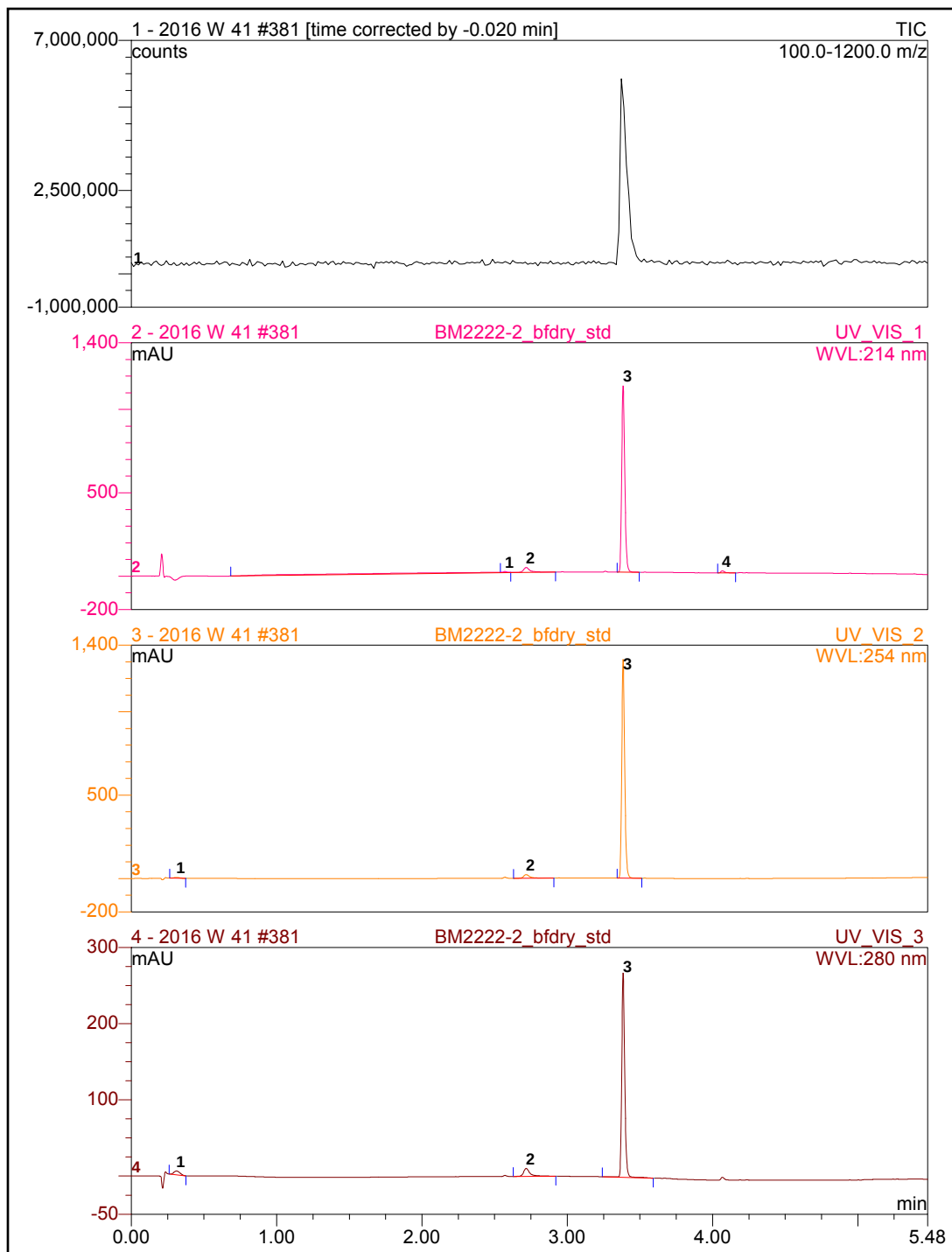
=====
*** End of Report ***
=====

Compound 50

Operator:service-thermo Timebase:INDIA Sequence:2016 W 41

Page 1-4
10/14/2016 2:10 PM

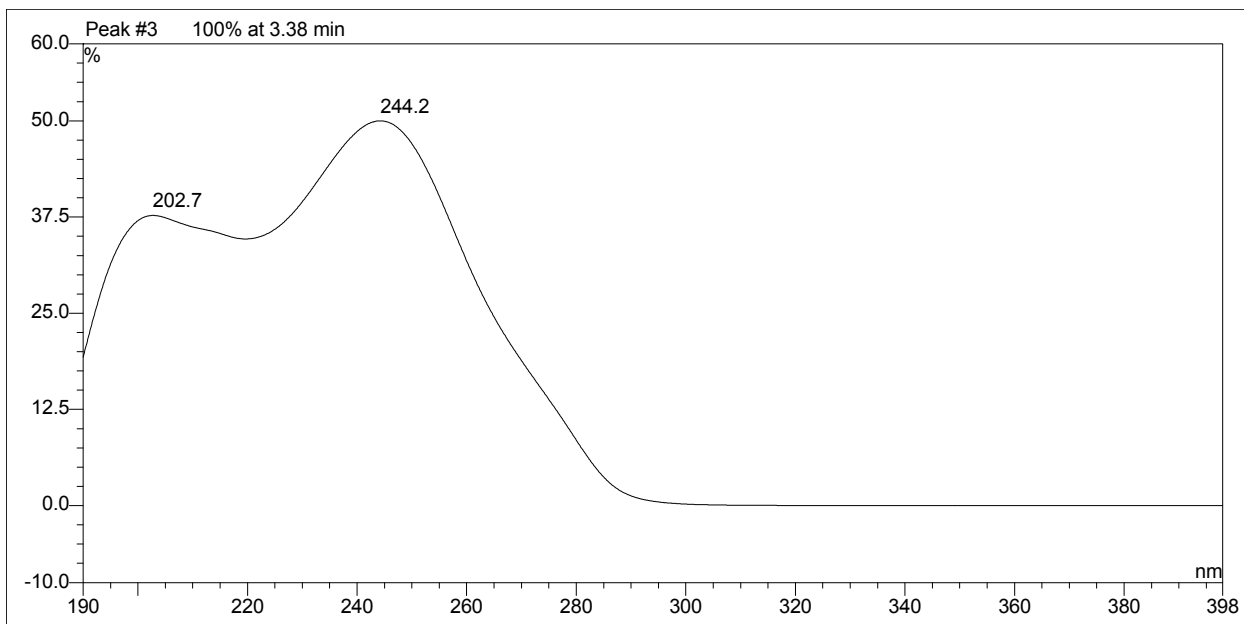
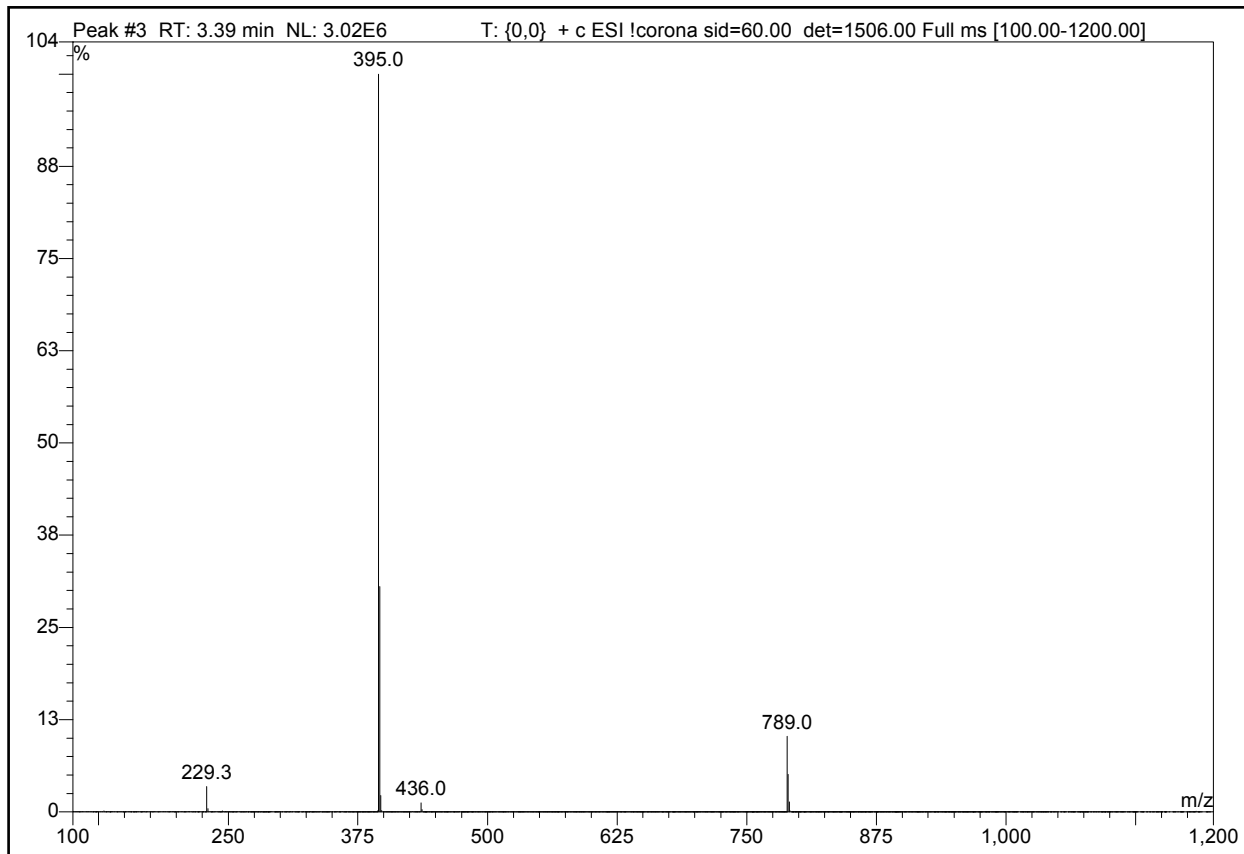
Sample Name: BM2222-2_bfdry_std **Injection Volume:** 1.0 uL
Control Program: Purity 5 min 5-100% positive **UserID:** Johanna
Recording Time: 10/14/2016 10:28



Highest m/z responses								
No.	Ret.Time min	Height mAU	Area mAU*min	Rel.Area %	Mass - 1 m/z	Mass - 2 m/z	Mass - 3 m/z	
1	0.31	4.724	0.223	0.69	101	119	105	
2	2.72	21.440	1.089	3.36	196	224	130	
3	3.38	1311.585	31.086	95.95	395	396	789	

Sample Name: BM2222-2_bfdry_std
Control Program Purity 5 min 5-100% positive
Recording Time:#####

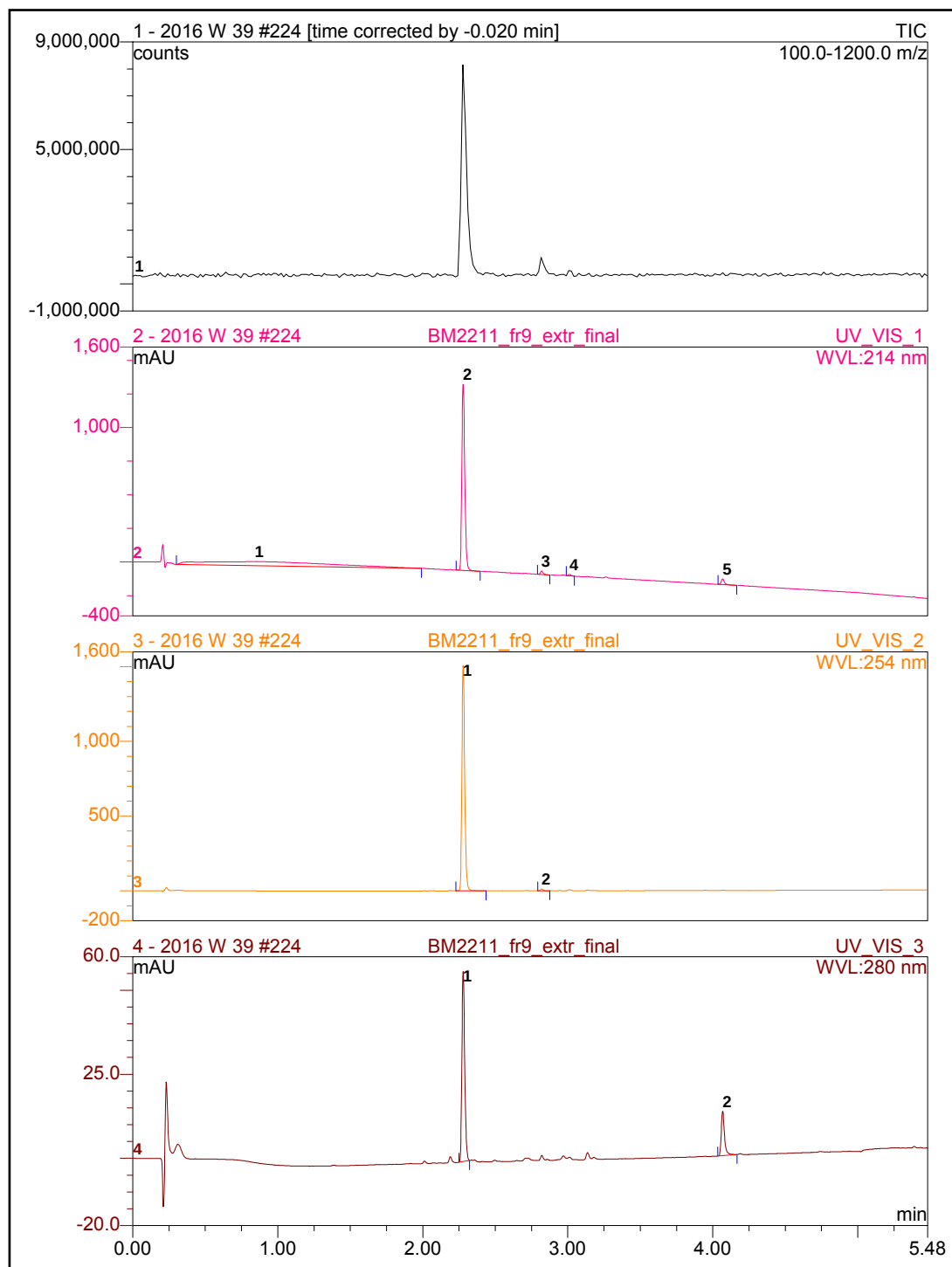
Injection Volume: 1.0 μ L
UserID Johanna



Compound 51

Sample Name: BM2211_fr9_extr_final
Control Program: Purity 5 min 5-100% positive
Recording Time: 9/29/2016 11:33

Injection Volume: 2.0 uL
UserID Johanna

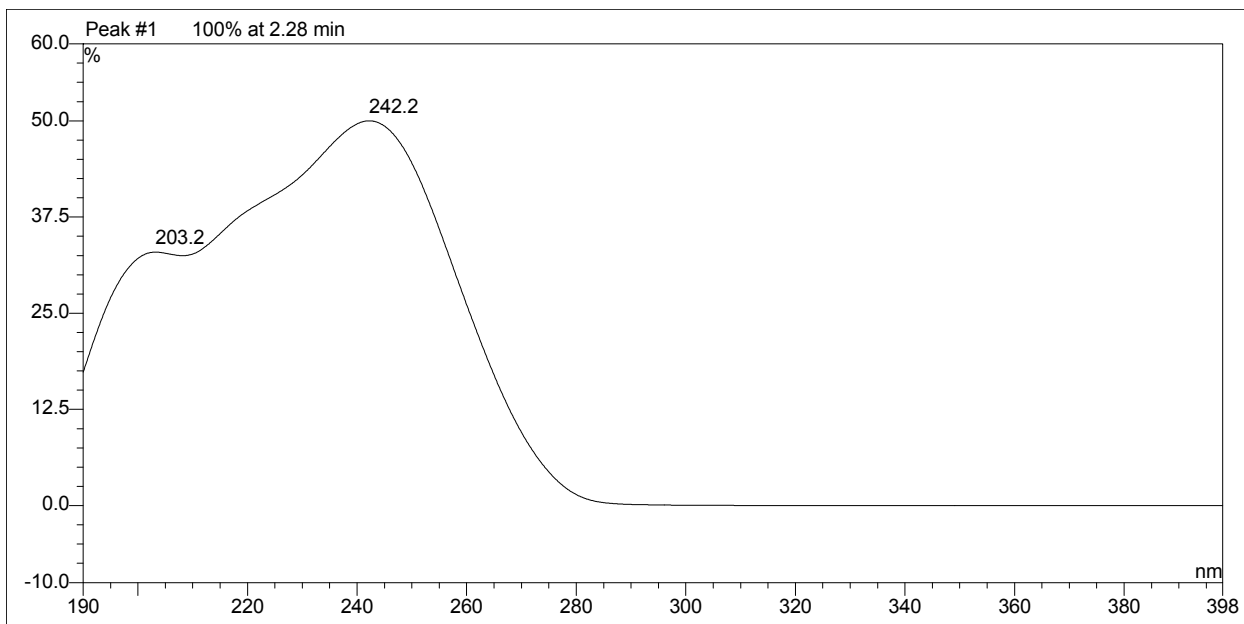
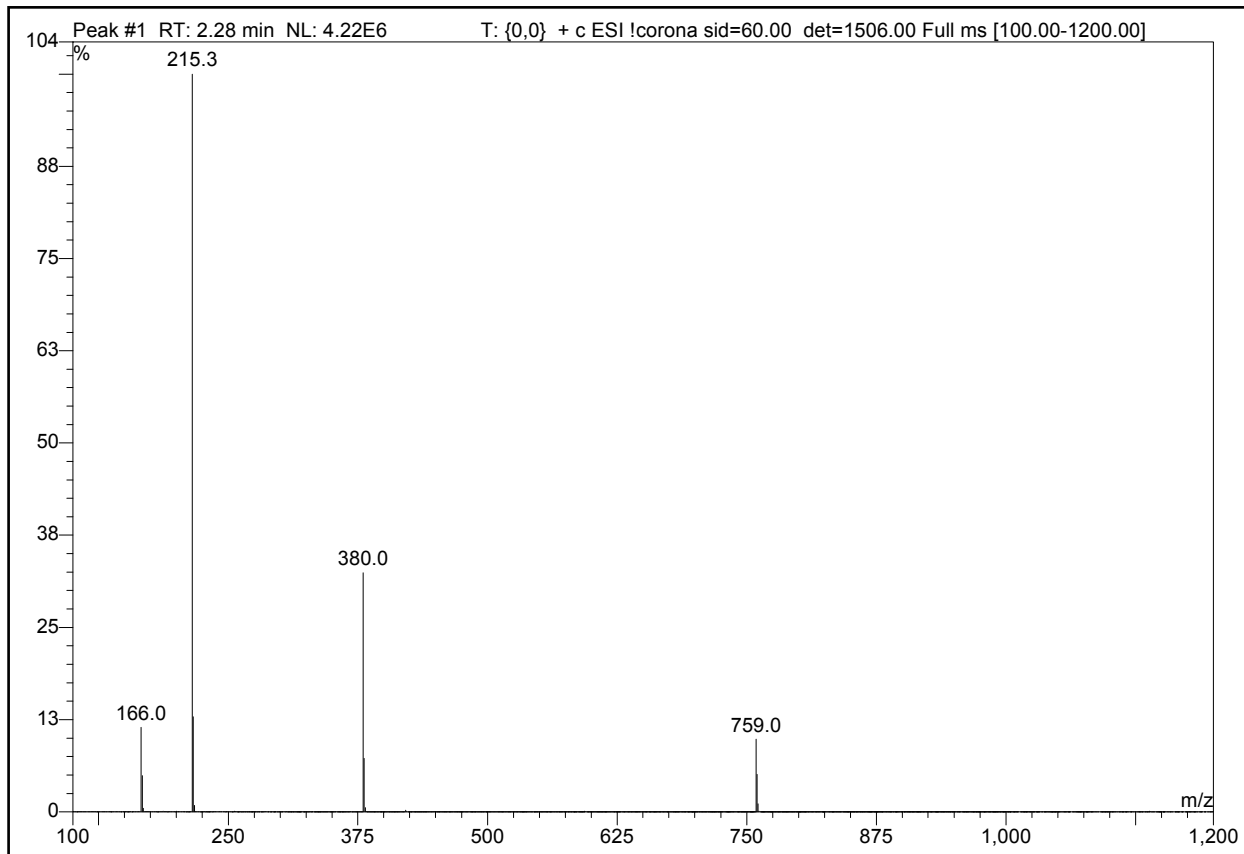


Highest m/z responses

No.	Ret.Time min	Height mAU	Area mAU*min	Rel.Area %	Mass - 1 m/z	Mass - 2 m/z	Mass - 3 m/z
1	2.28	1508.731	33.672	99.20	215	380	216
2	2.82	12.428	0.271	0.80	215	336	280

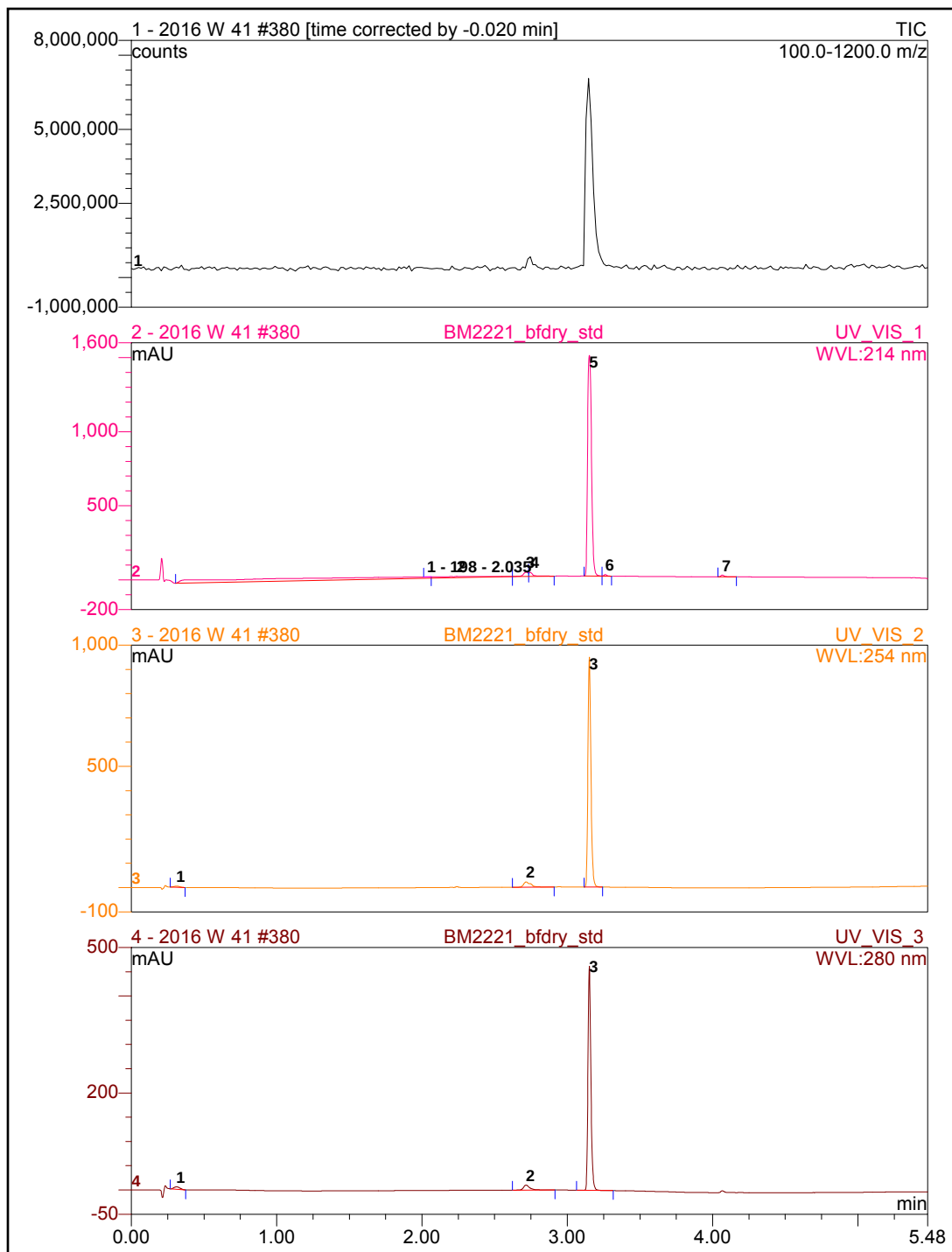
Sample Name: BM2211_fr9_extr_final
Control Program Purity 5 min 5-100% positive
Recording Time: 9/29/2016 11:33

Injection Volume: 2.0 μ L
UserID Johanna



Sample Name: BM2221_bfdry_std
Control Program: Purity 5 min 5-100% positive
Recording Time: 10/14/2016 10:21

Injection Volume:	1.0 uL
UserID	Johanna

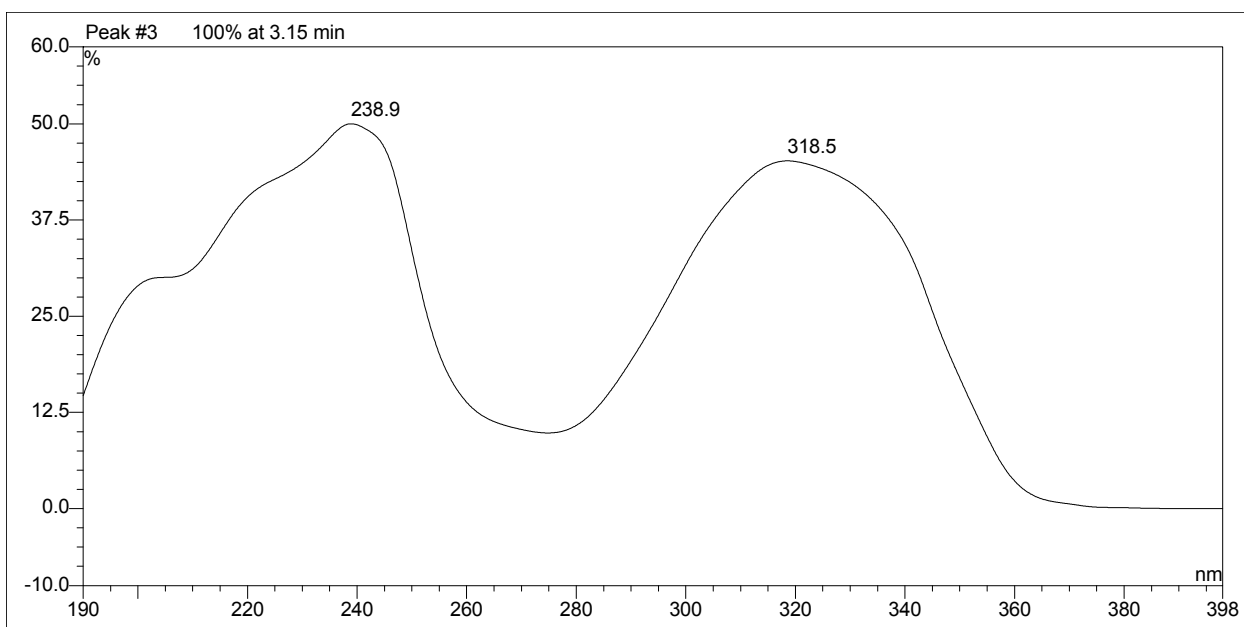
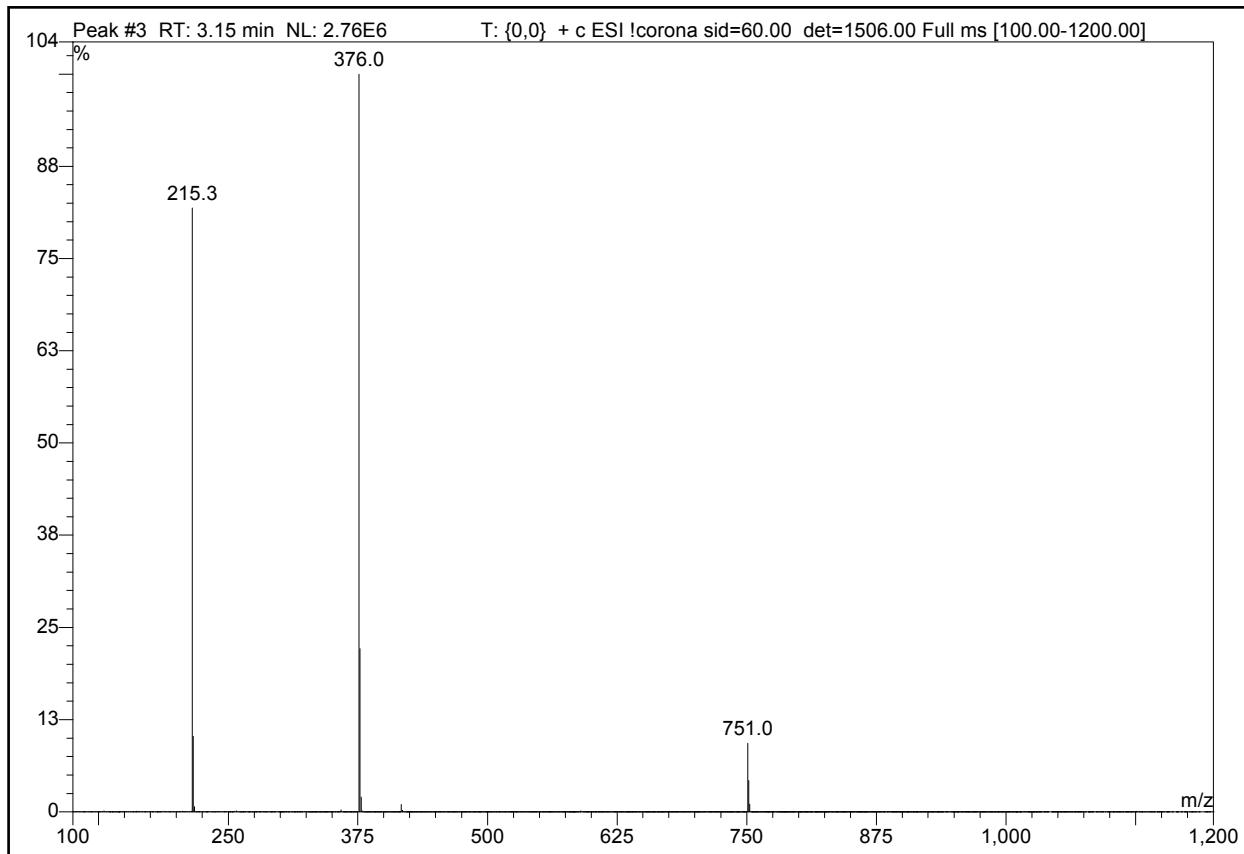


Total purity ignoring the integration of the void:
Purity @254 nM is
 $22518 / (22518 + 1284) = 95\%$

Highest m/z responses							
No.	Ret.Time min	Height mAU	Area mAU*min	Rel.Area %	Mass - 1 m/z	Mass - 2 m/z	Mass - 3 m/z
1	0.31	4.631	0.216	0.90	121	111	117
2	2.72	21.645	1.284	5.35	196	126	109
3	3.15	948.632	22.518	93.75	376	215	377

Sample Name: BM2221_bfdry_std
Control Program Purity 5 min 5-100% positive
Recording Time:#####

Injection Volume: 1.0 uL
UserID Johanna



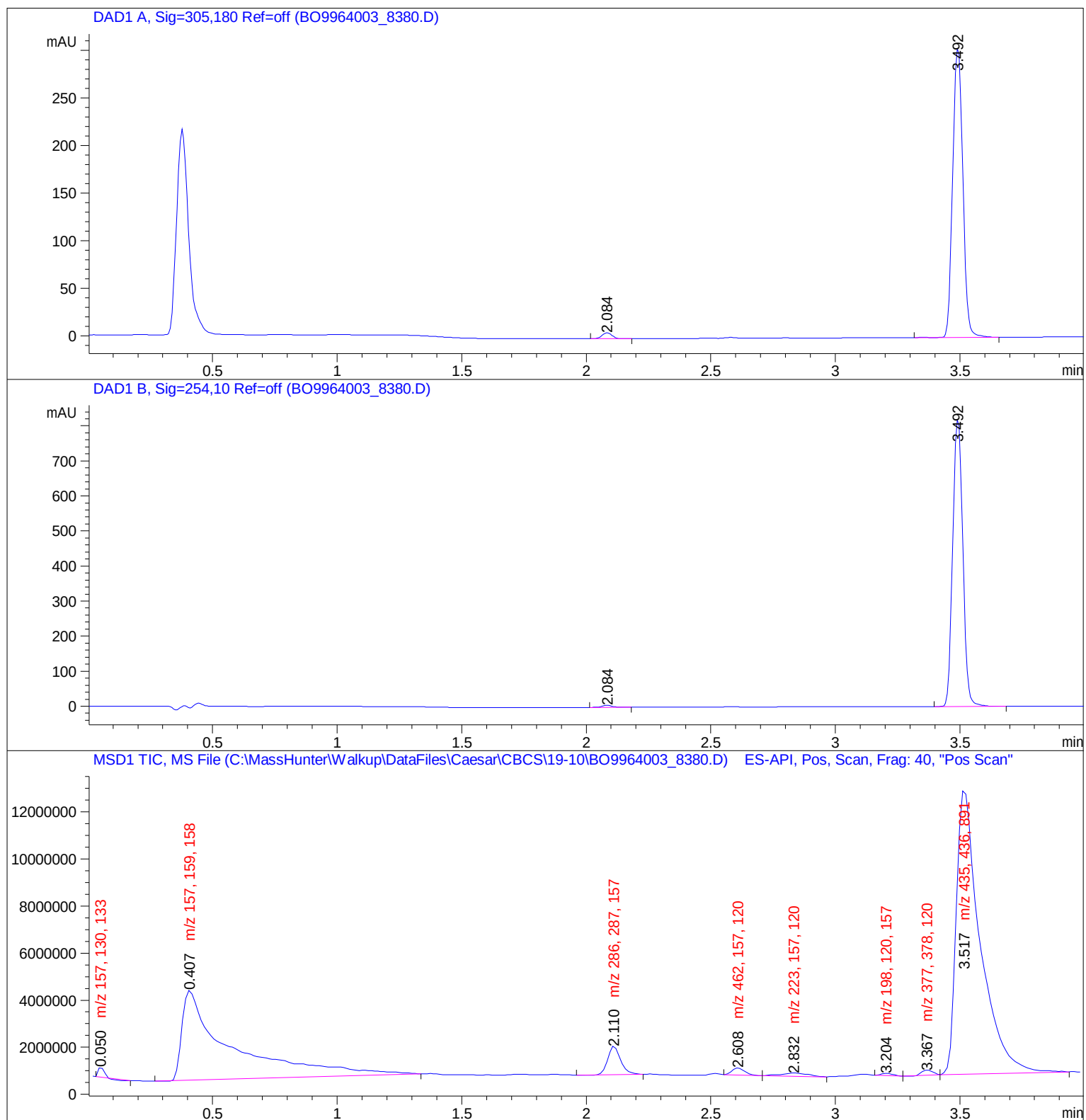
Sample Name: B09964003

Compound 53

```
=====
Acq. Operator   : Administrator
Sample Operator : Martin Haraldsson
Acq. Instrument : Caesar                      Location :   D1B-E3
Injection Date  : 10/24/2019 3:02:10 PM      Inj       :    1
                                           Inj Volume : Inj prog
Method          : C:\Users\Public\Documents\ChemStation\1\Methods\X1097-3.M
Last changed    : 10/24/2019 3:00:25 PM by Administrator
                  (modified after loading)
Method Info     : X-bridge C18, 50x3.0 mm, 3.5u, 10-97% MeCN 3min,1ml/min, B: MeCN C: NH4HC03

Sample Info     : Walkup method: 'X1097-3'
                  Target:
```

Sample Name: B09964003



=====
Area Percent Report
=====

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000
Do not use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=305,180 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.084	BB	0.0482	18.05229	6.16036	2.0525
2	3.492	BB	0.0449	861.49139	305.33118	97.9475

Totals : 879.54369 311.49154

Signal 2: DAD1 B, Sig=254,10 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.084	BB	0.0478	17.48800	6.02968	0.7485
2	3.492	BB	0.0449	2319.05591	822.43872	99.2515

Totals : 2336.54391 828.46840

Signal 3: MSD1 TIC, MS File

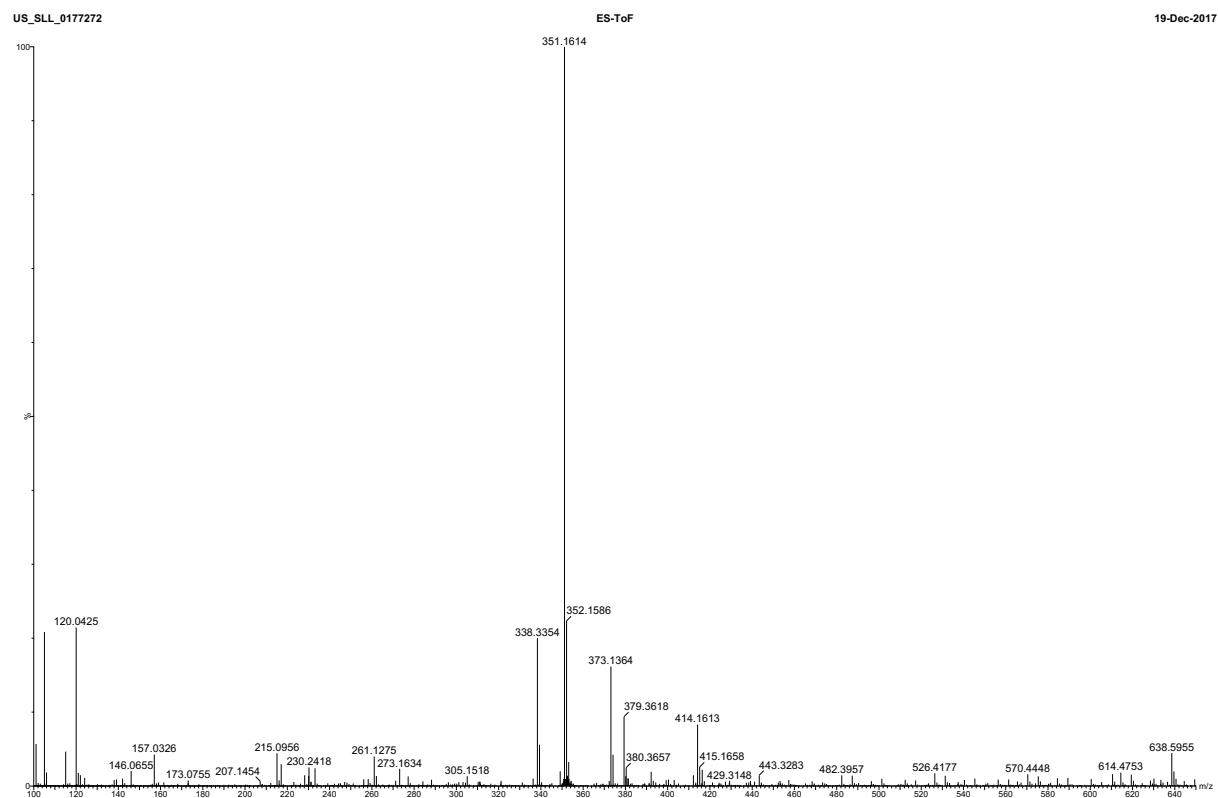
Peak #	RetTime [min]	Type	Width [min]	Area	Height	Area %
1	0.050	BB	0.0215	5.52340e5	4.28706e5	0.3931
2	0.407	BB	0.1767	5.18546e7	3.82792e6	36.9009
3	2.110	BB	0.0572	4.43920e6	1.22505e6	3.1590
4	2.608	BB	0.0527	1.09496e6	3.07905e5	0.7792
5	2.832	BB	0.0997	1.04669e6	1.43995e5	0.7448
6	3.204	BB	0.0592	3.22125e5	1.02086e5	0.2292
7	3.367	BB	0.0550	6.99770e5	2.24552e5	0.4980
8	3.517	BB	0.0957	8.05145e7	1.21939e7	57.2958

Totals : 1.40524e8 1.84541e7

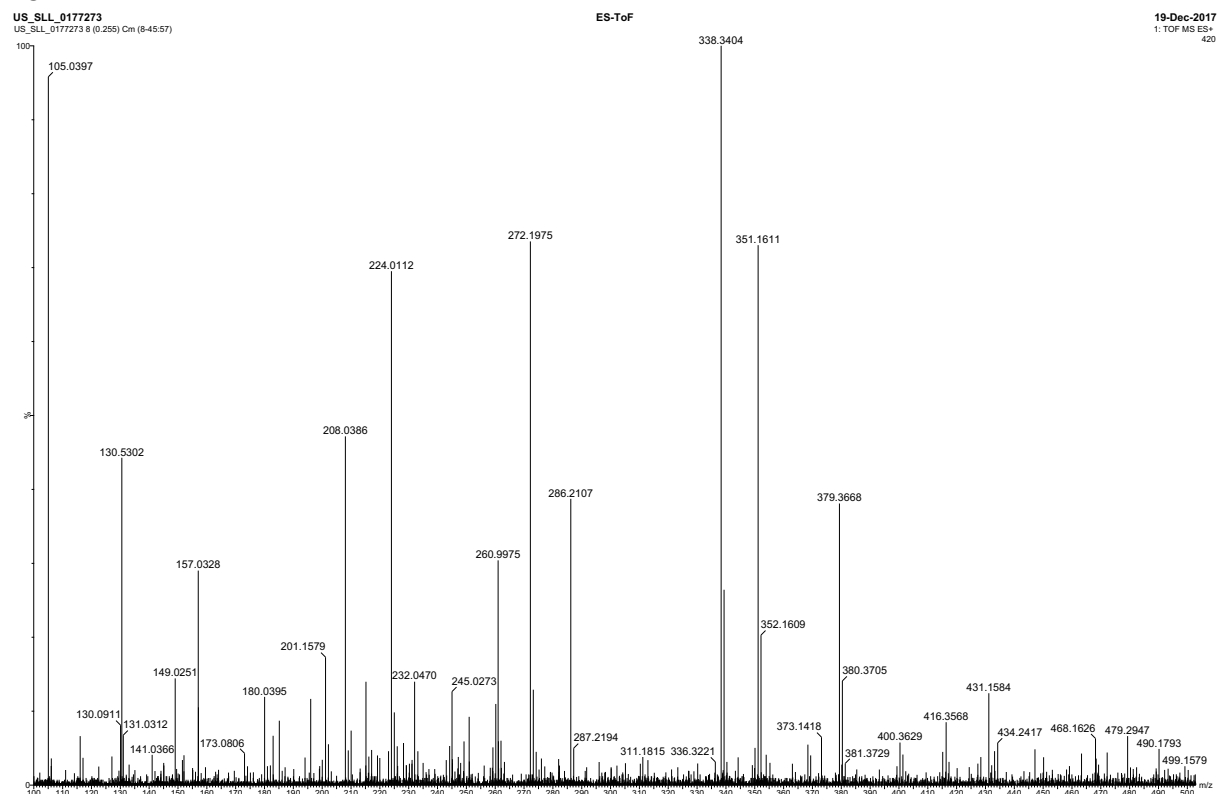
*** End of Report ***

HRMS Supporting Information

28



29

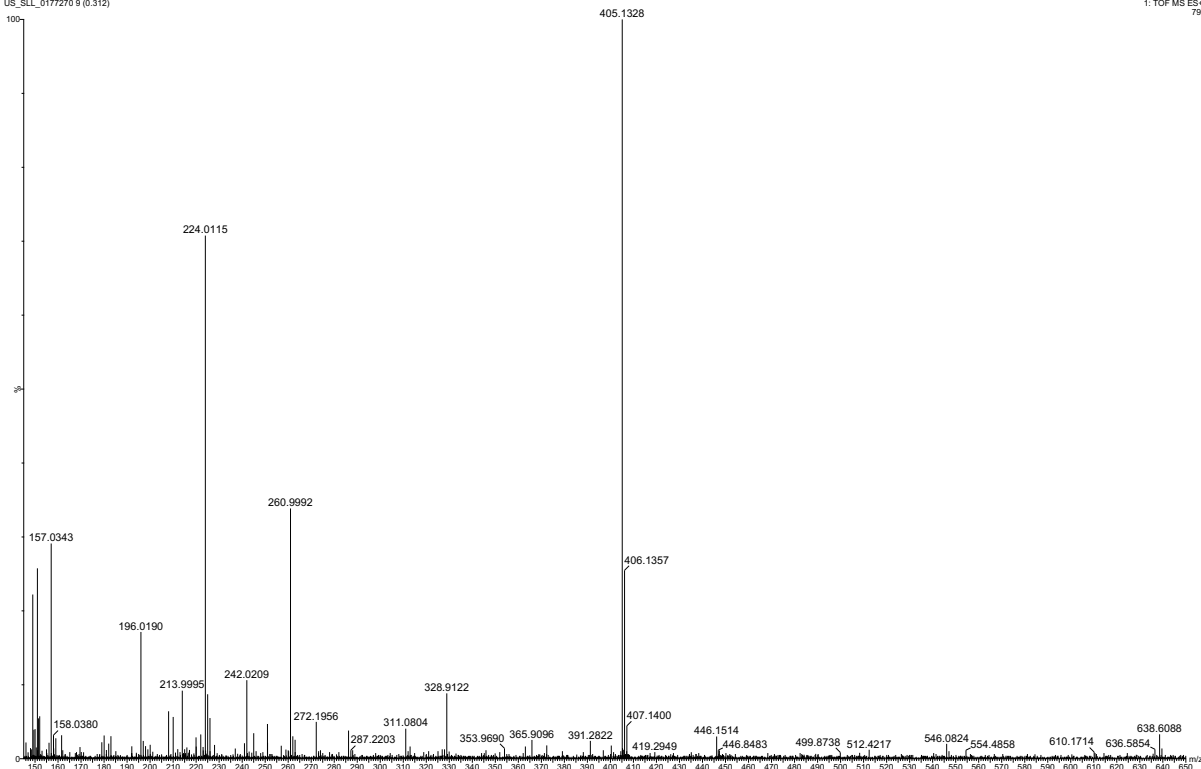


30

US_SLL_0177270
US_SLL_0177270.9 (0.312)

ES-ToF

19-Dec-2017
1: TOF MS ES+
798

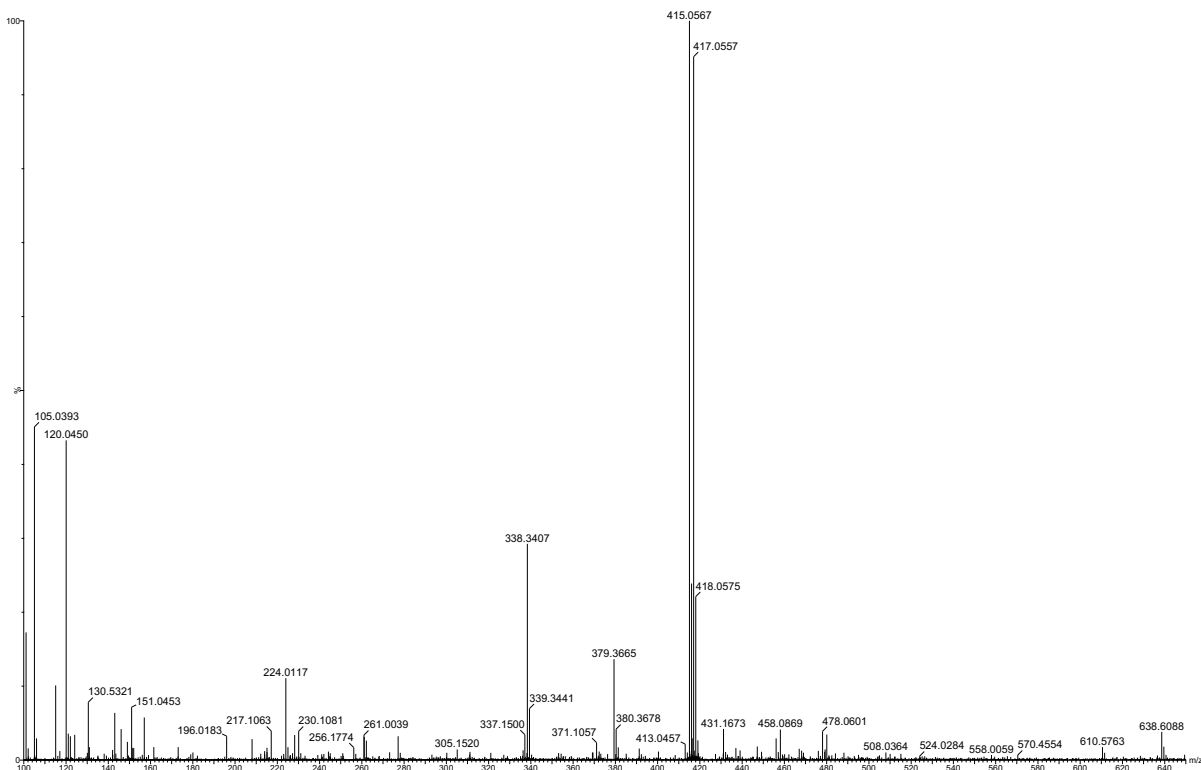


31

US_SLL_0177254

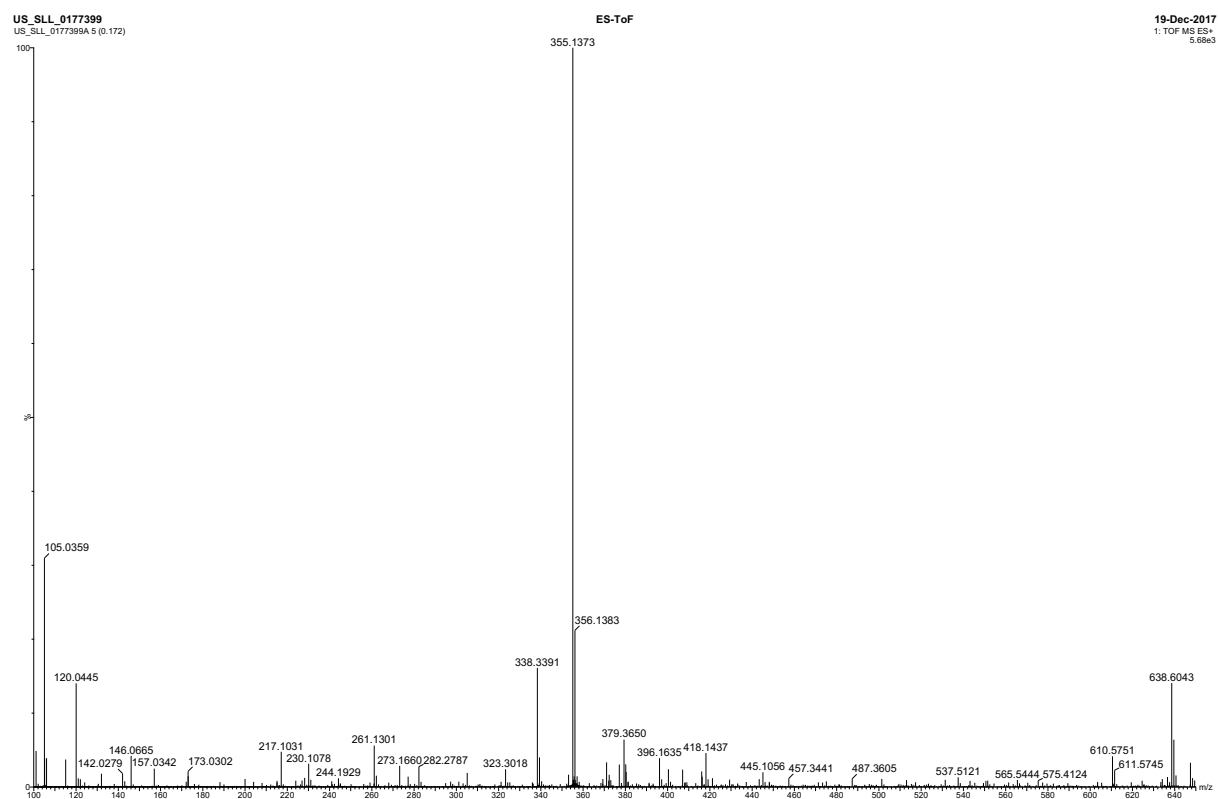
ES-ToF

19-Dec-2017

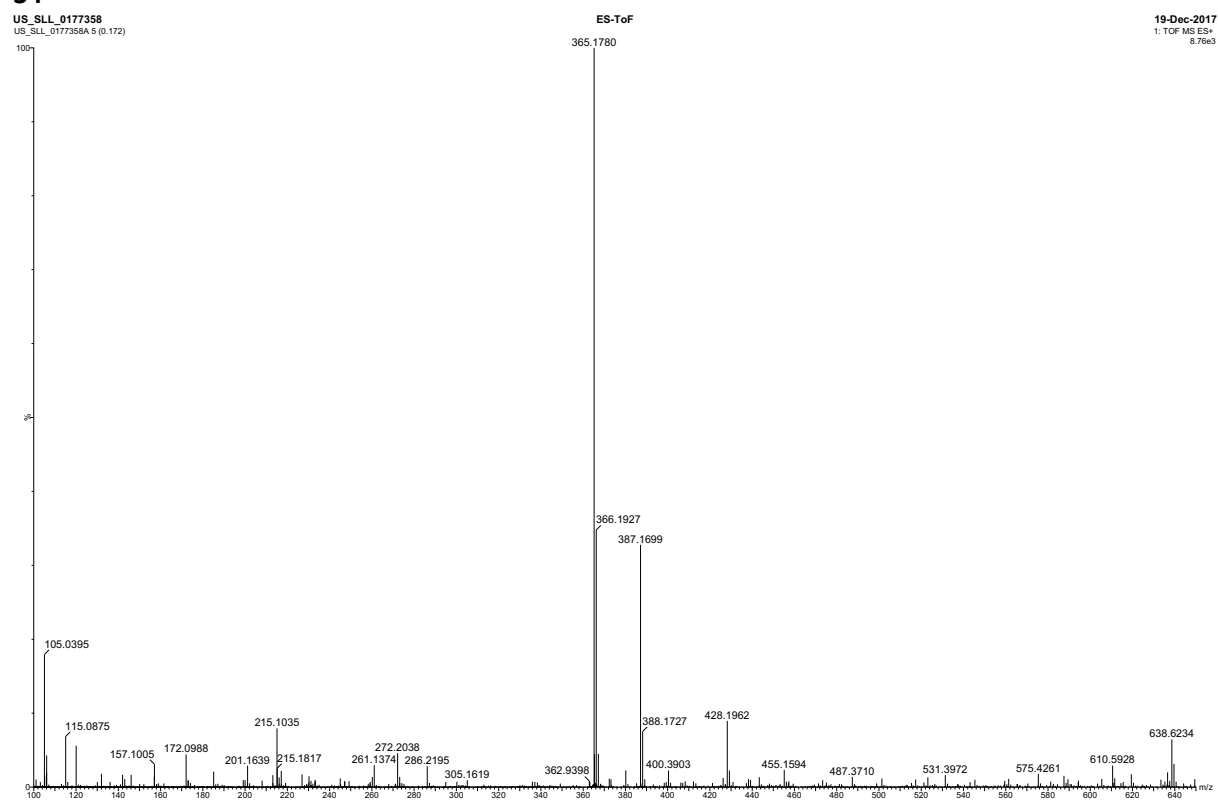


32 Data not available

33

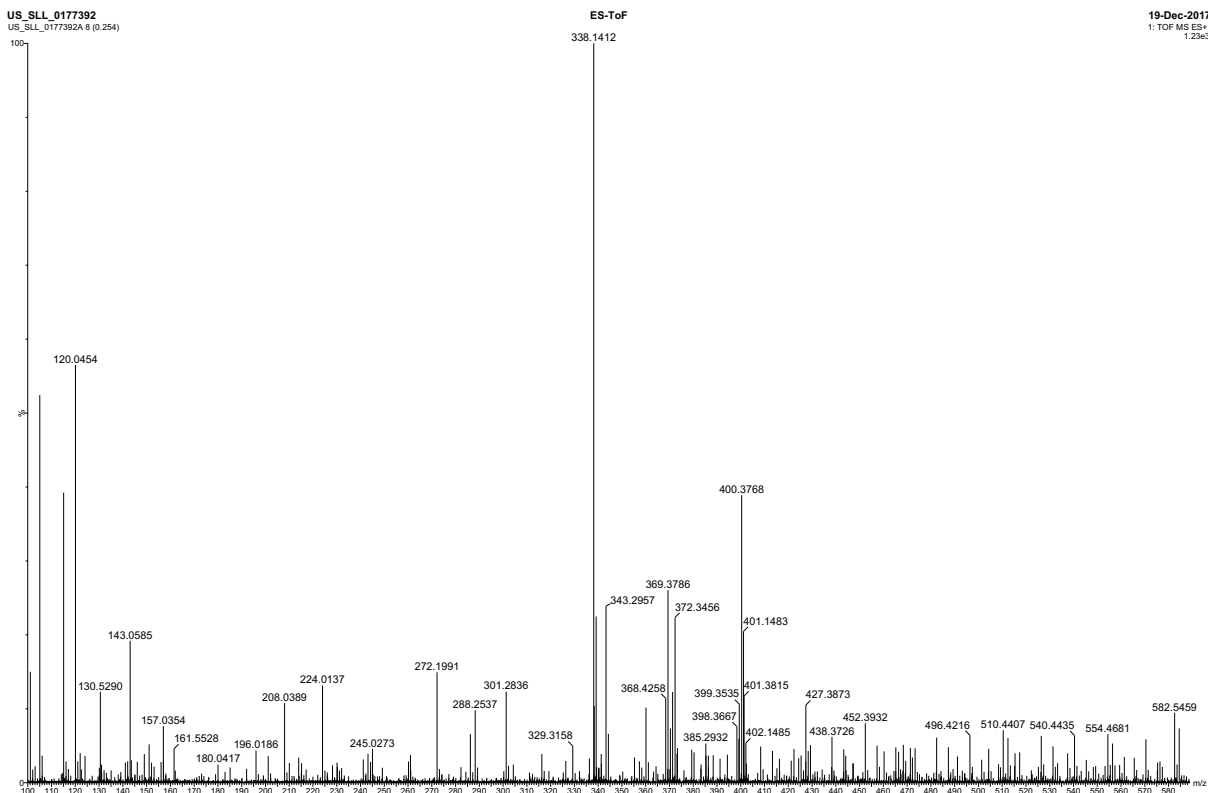


34

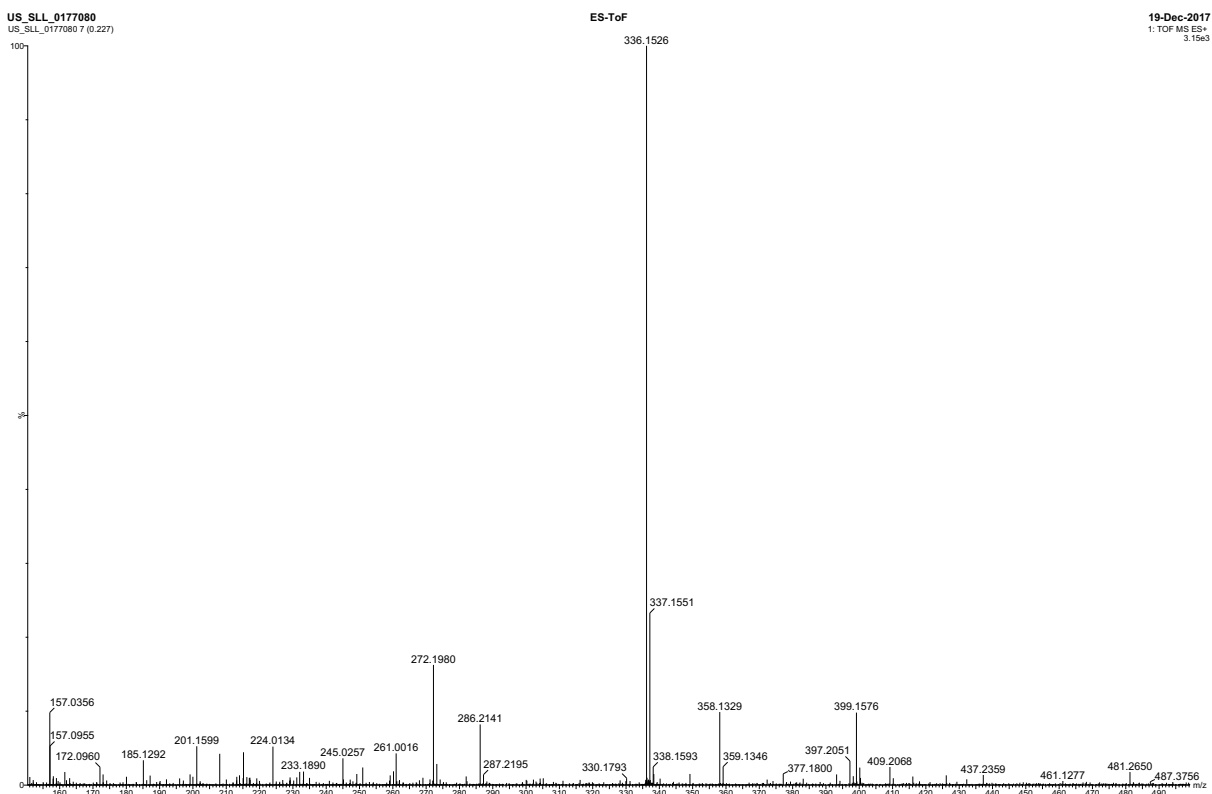


35 Data not available

36

US_SLL_0177392
US_SLL_0177392A.9 (0.254)

37

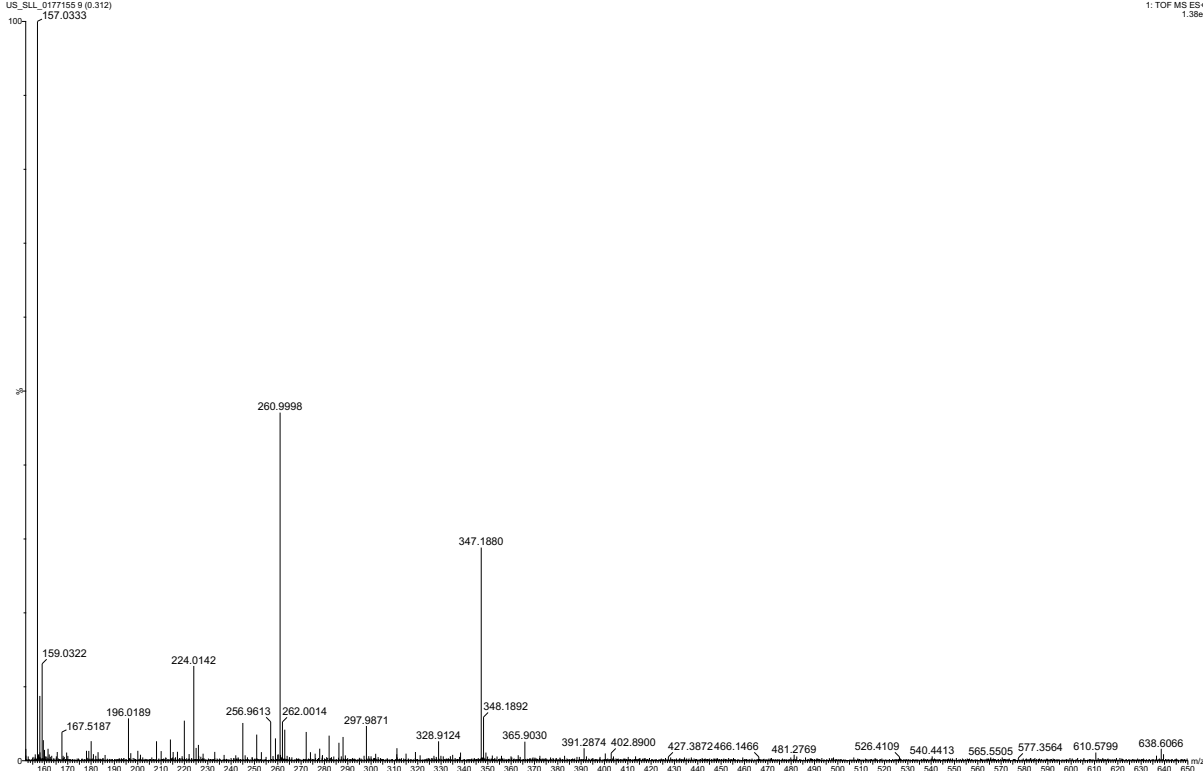
US_SLL_0177080
US_SLL_0177080.7 (0.227)

38

US_SLL_0177155
US_SLL_0177155.9 (0.312)

ES-ToF

19-Dec-2017
1: TOF MS ES+
1.38e3

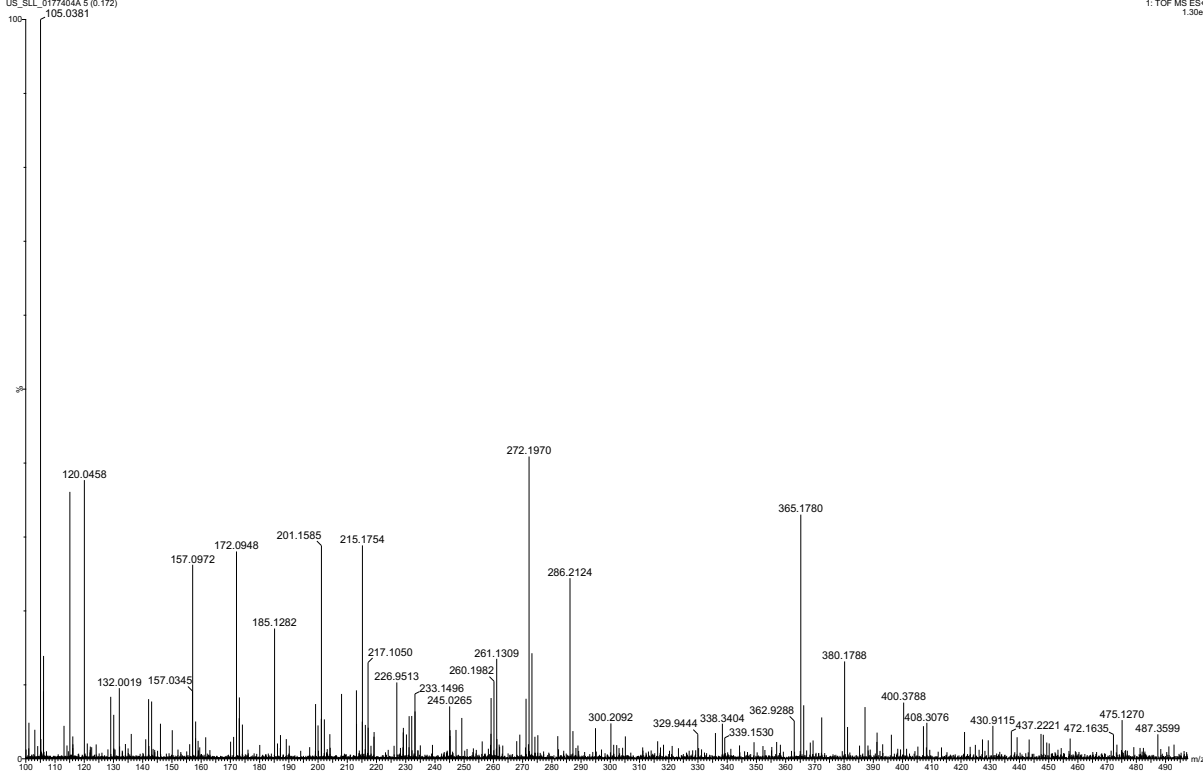


39

US_SLL_0177404
US_SLL_0177404.5 (0.172)

ES-ToF

19-Dec-2017
1: TOF MS ES+
1.30e3

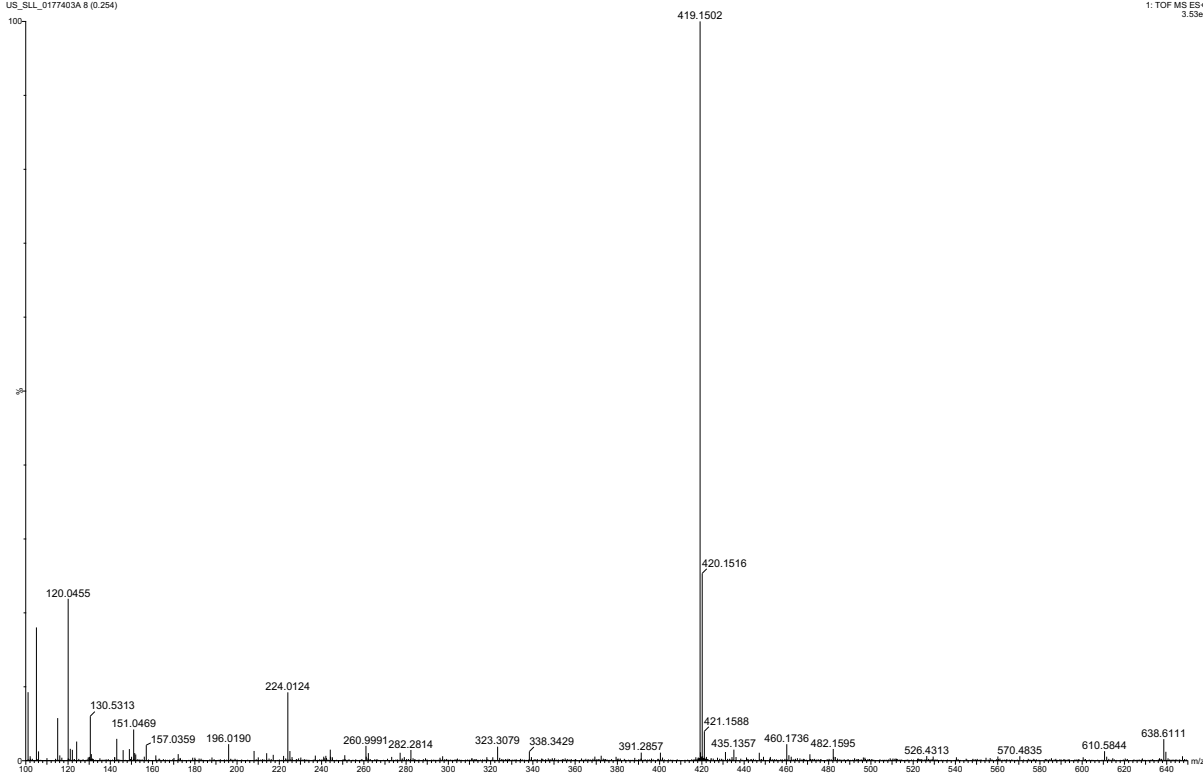


40

US_SLL_0177403
US_SLL_0177403A.9 (0.254)

ES-ToF

19-Dec-2017
1: TOF MS ES+
3.53e3

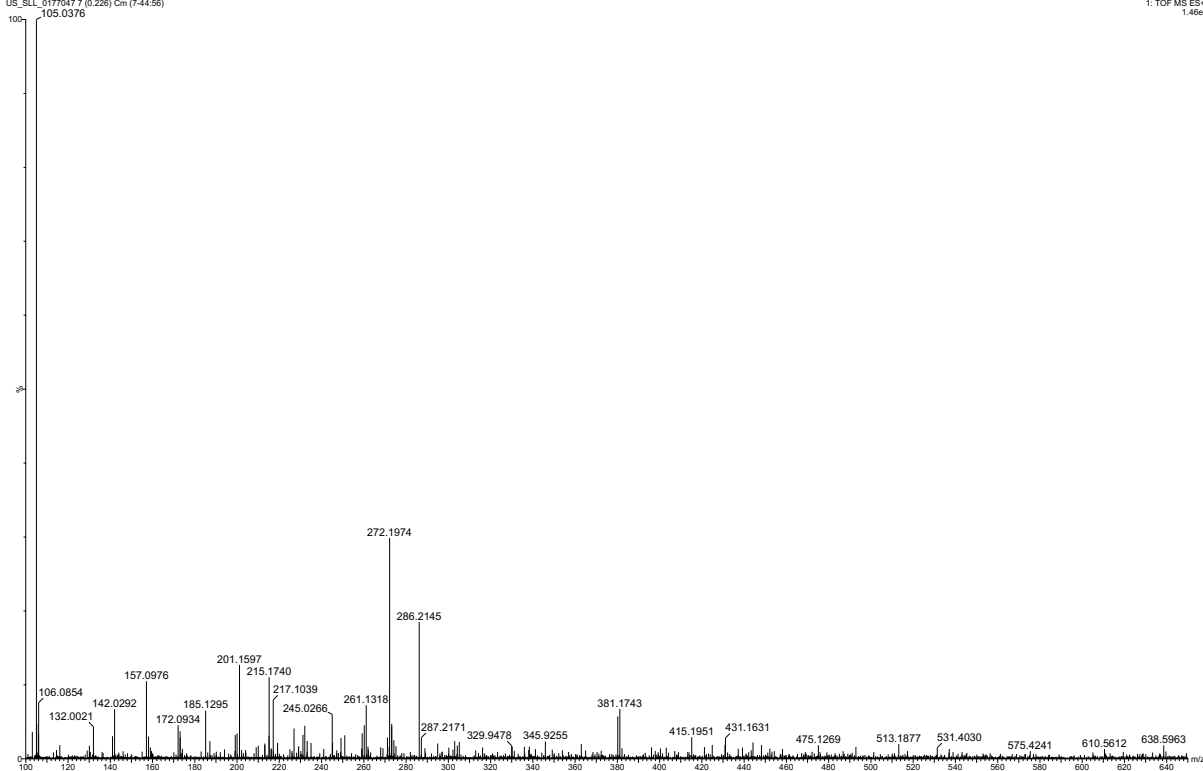


41

US_SLL_0177047
US_SLL_0177047.7 (0.226) Cm (7.44:56)

ES-ToF

19-Dec-2017
1: TOF MS ES+
1.46e3

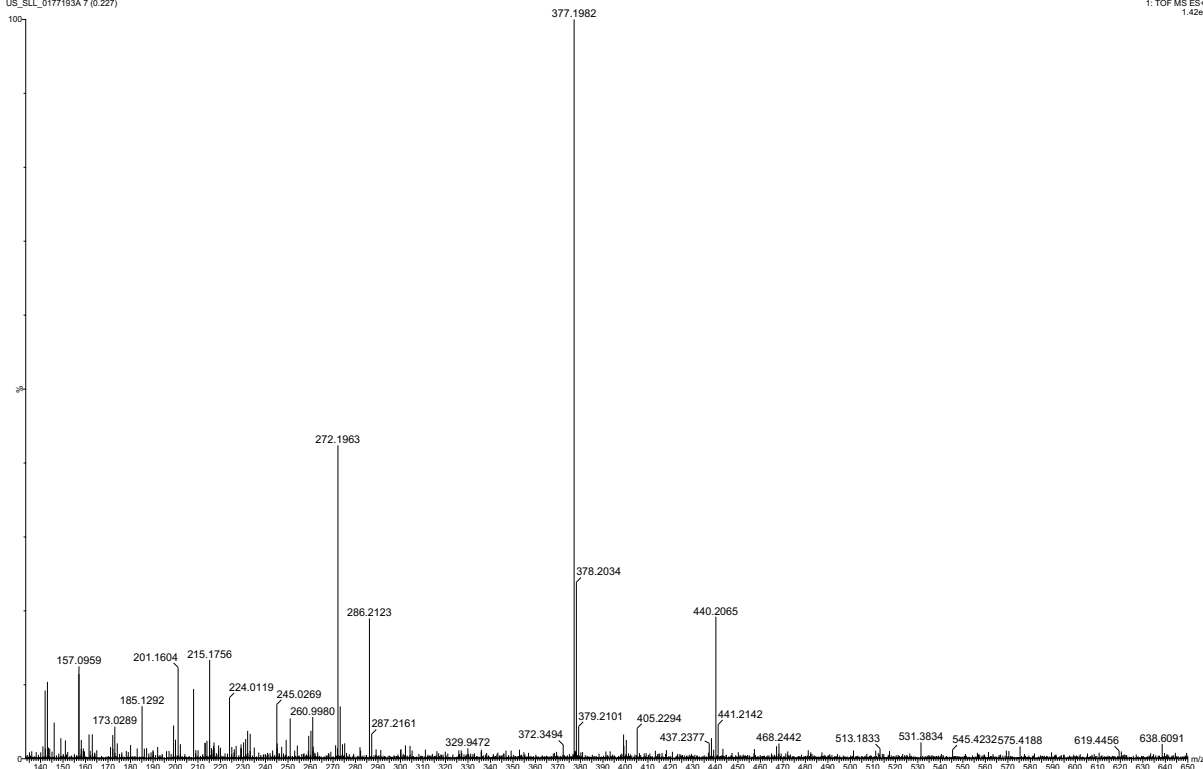


42 Data not available

43

US_SLL_0177193
US_SLL_0177193A.7 (0.227)

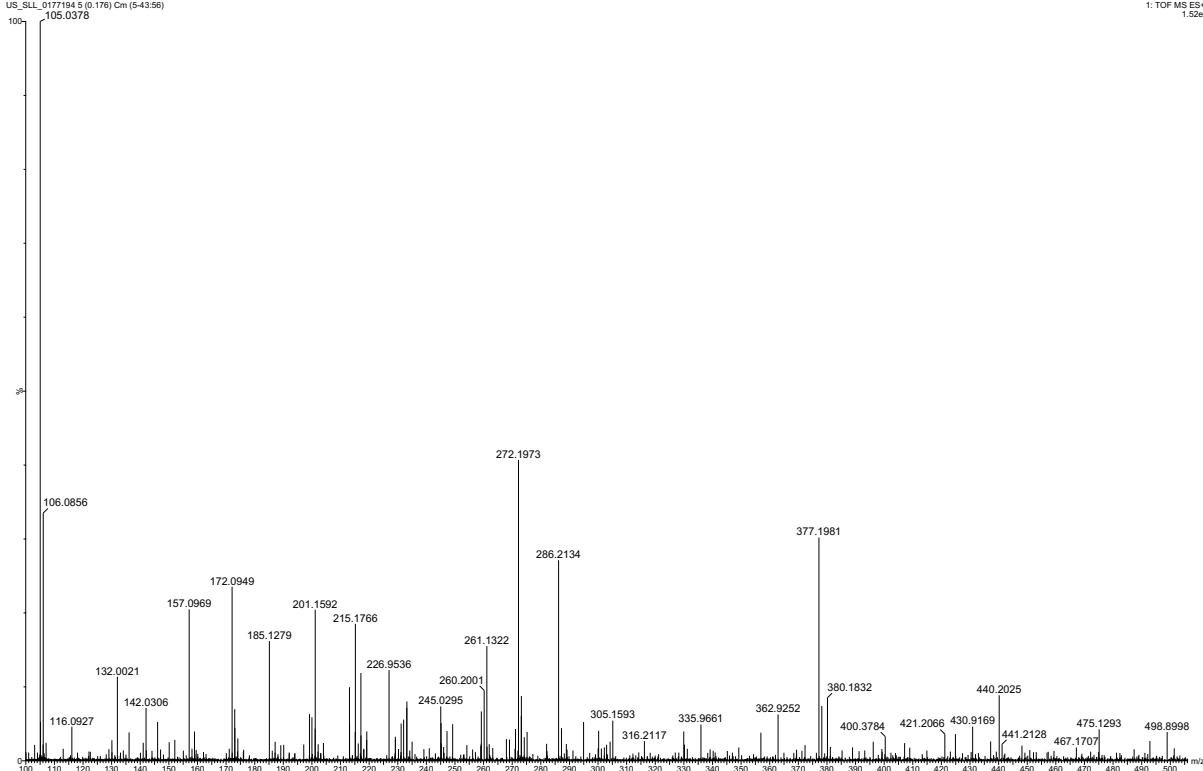
ES-ToF

19-Dec-2017
1: TOF MS ES+
1.42e3

44

US_SLL_0177194
US_SLL_0177194.5 (0.176) Cm (5-43.56)

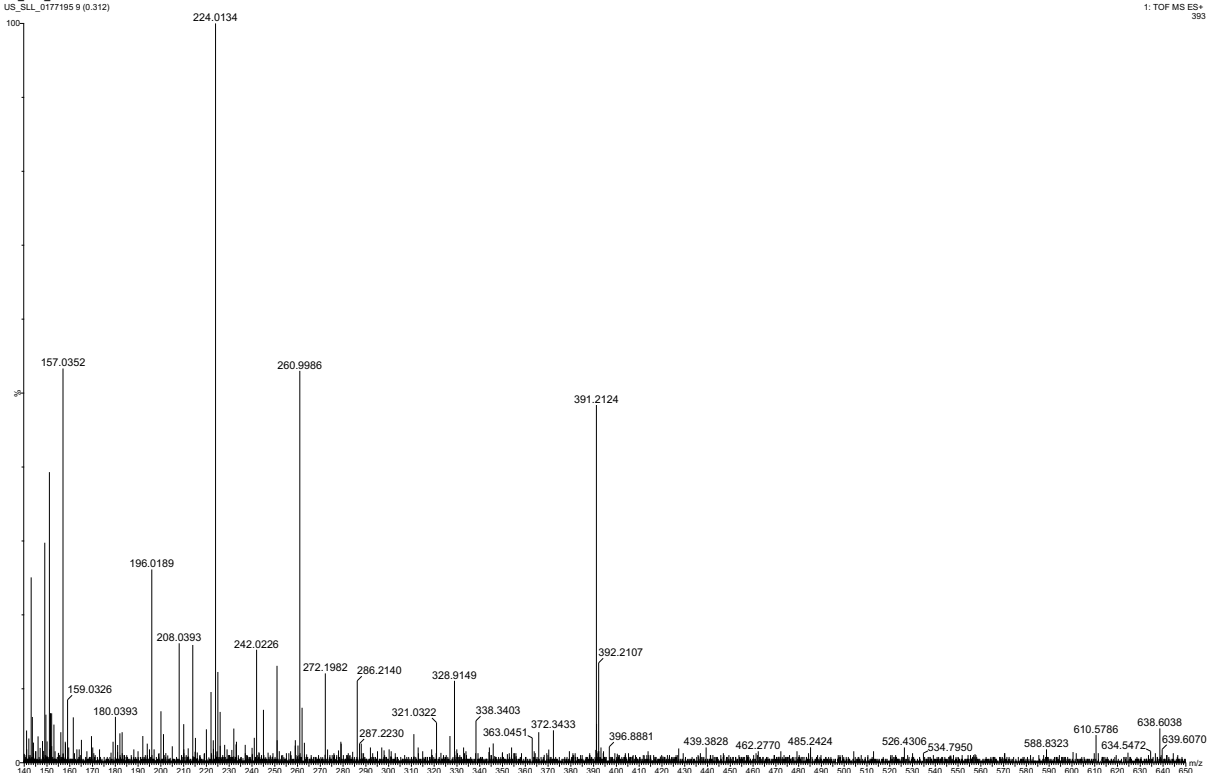
ES-ToF

19-Dec-2017
1: TOF MS ES+
1.52e3

45

US_SLL_0177195
US_SLL_0177195 9 (0.312)

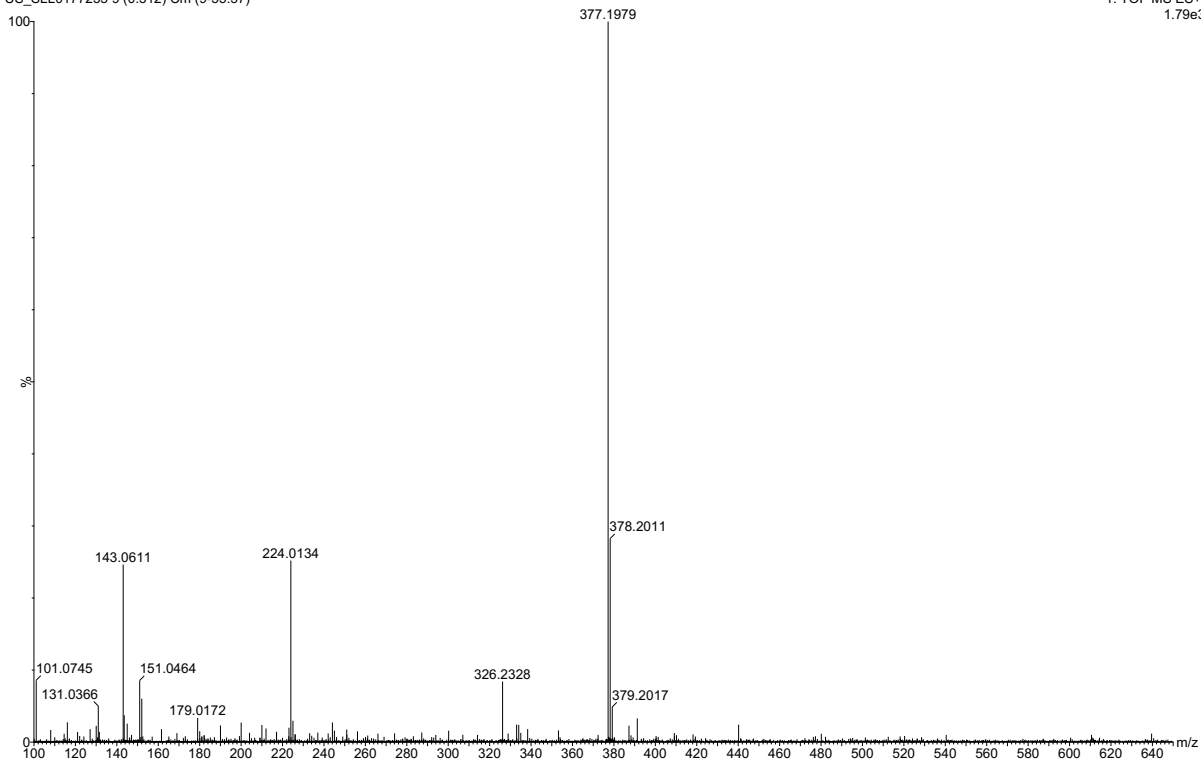
ES-ToF

19-Dec-2017
1: TOF MS ES+
393

46

US_SLL0177235
US_SLL0177235 9 (0.312) Cm (9-55:57)

ES-ToF

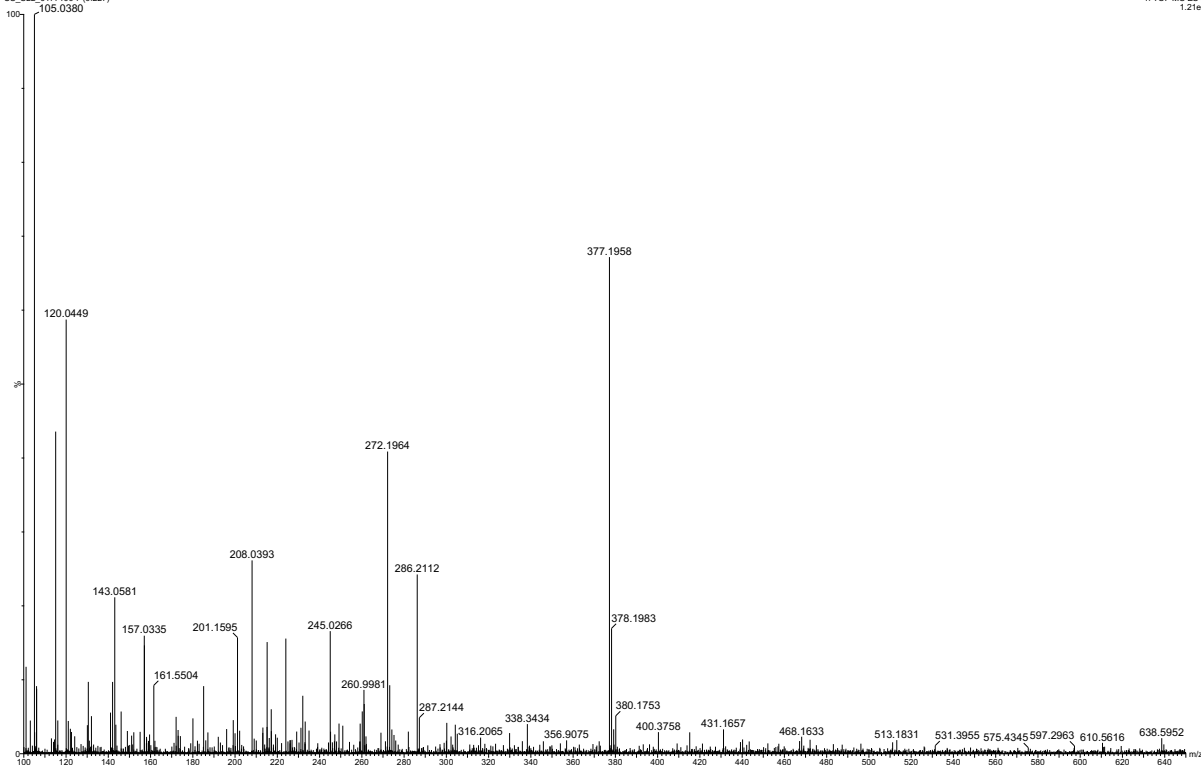
11-Dec-2018
1: TOF MS ES+
1.79e3

47

US_SLL_0177100
US_SLL_0177100 7 (0.227)
105.0380

ES-ToF

19-Dec-2017
1: TOF MS ES+
1.21e3

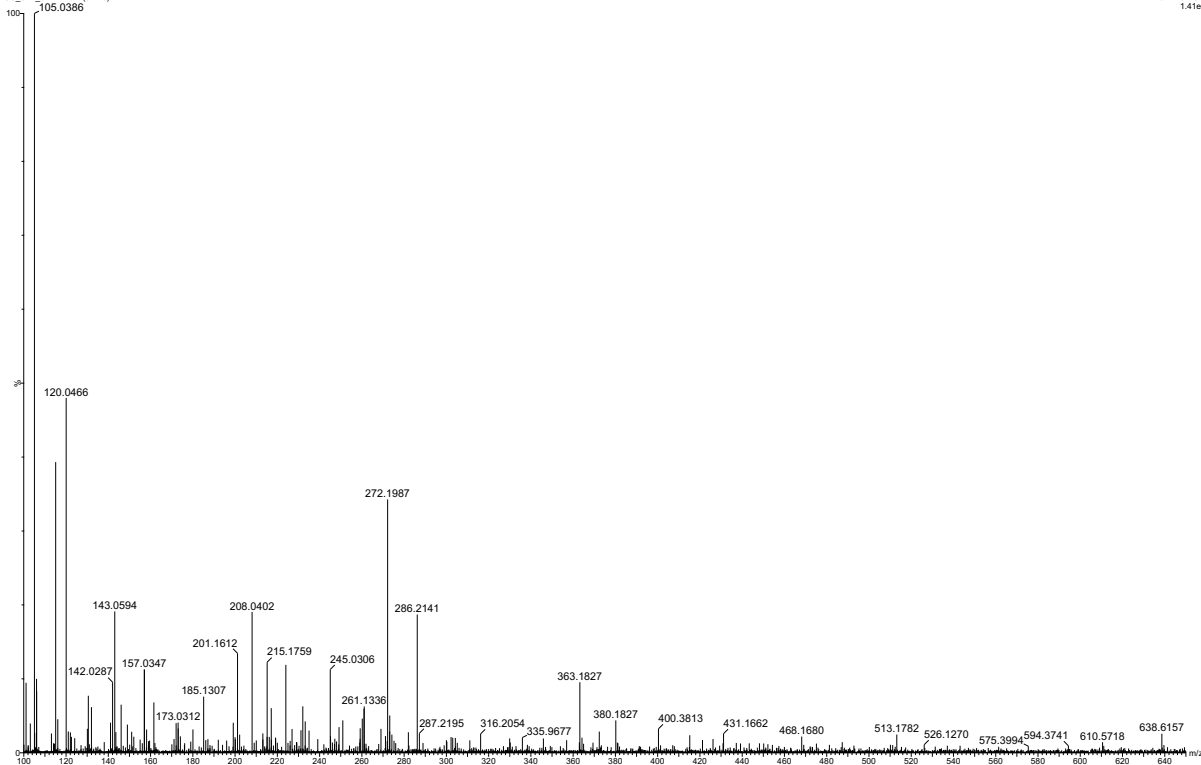


48

US_SLL_0177113
US_SLL_0177113 7 (0.226)
105.0386

ES-ToF

19-Dec-2017
1: TOF MS ES+
1.41e3

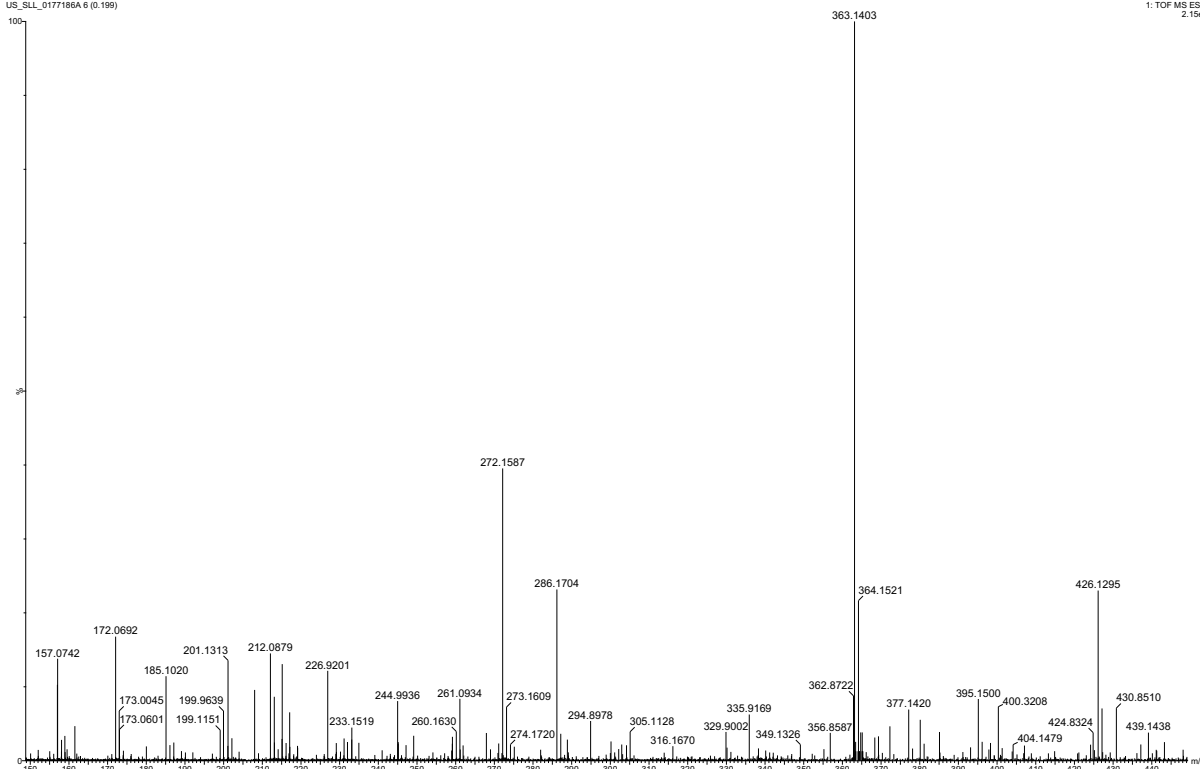


49

US_SLL_0177186
US_SLL_0177186A 6 (0.199)

ES-ToF

19-Dec-2017
1: TOF MS ES+
2.15e3

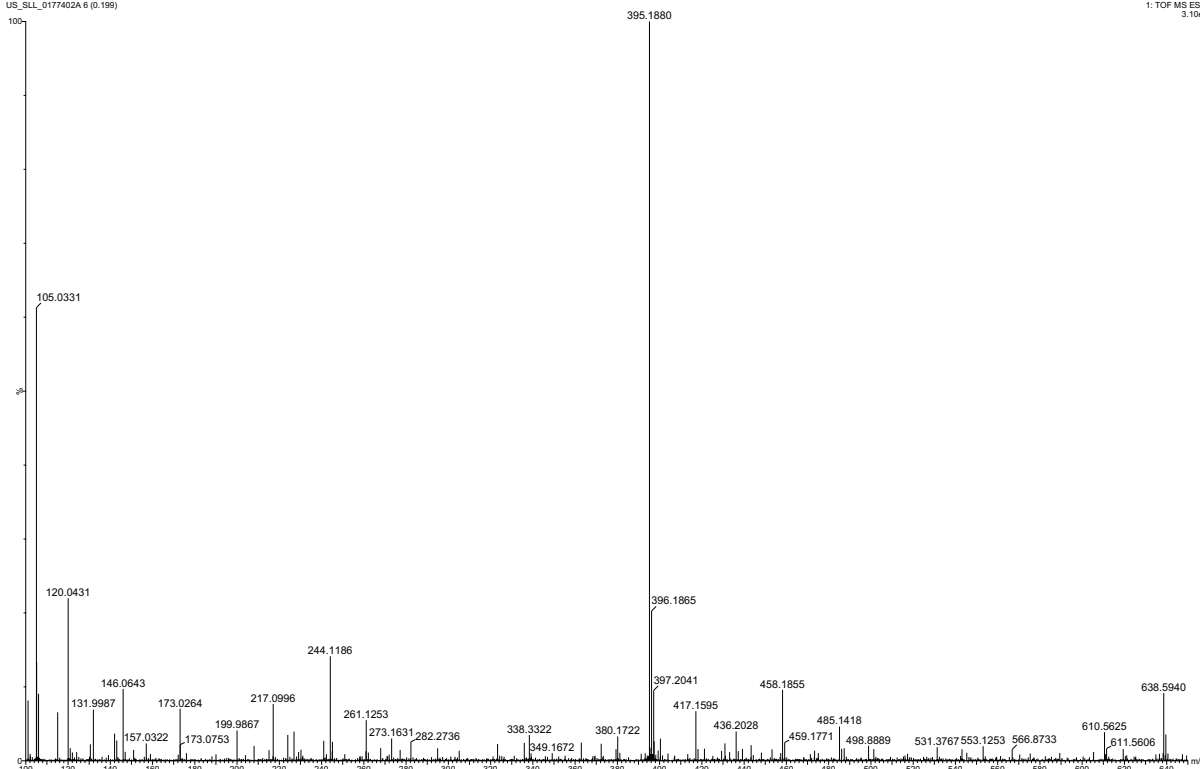


50

US_SLL_0177402
US_SLL_0177402A 6 (0.199)

ES-ToF

19-Dec-2017
1: TOF MS ES+
3.10e3

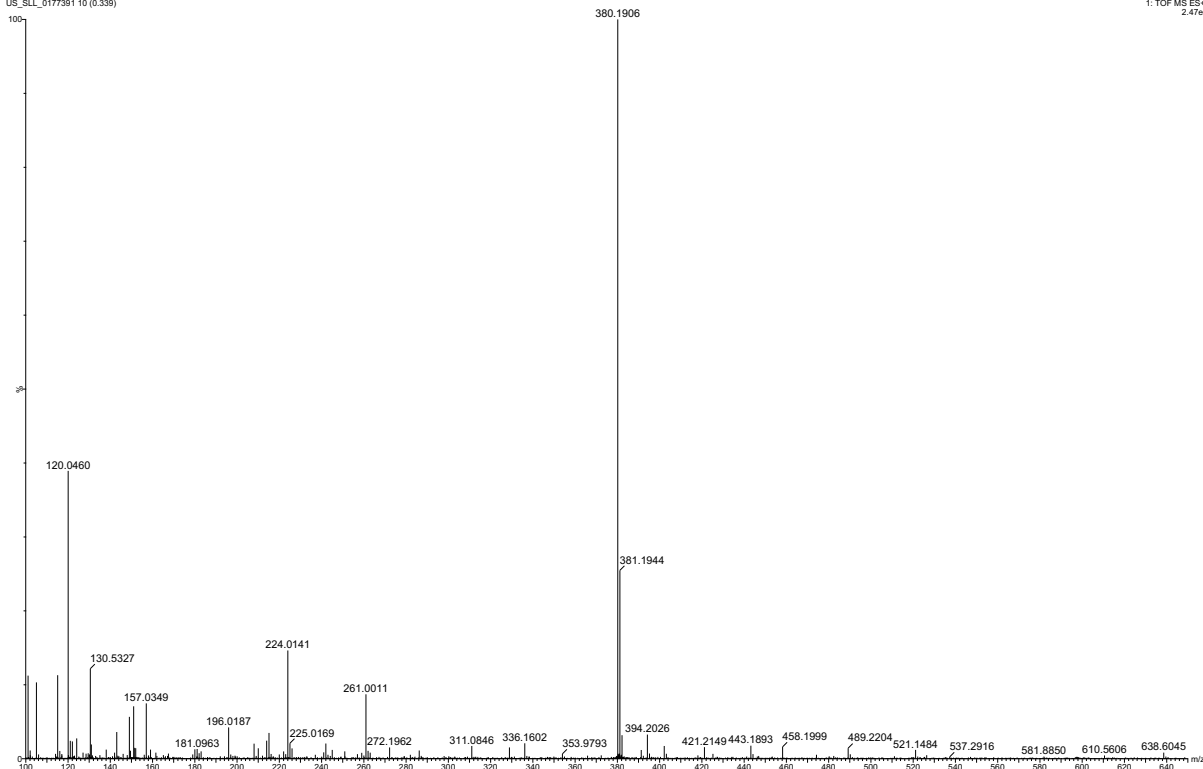


51

US_SLL_0177391
US_SLL_0177391.10 (0.339)

ES-ToF

19-Dec-2017
1: TOF MS ES+
2.47e3

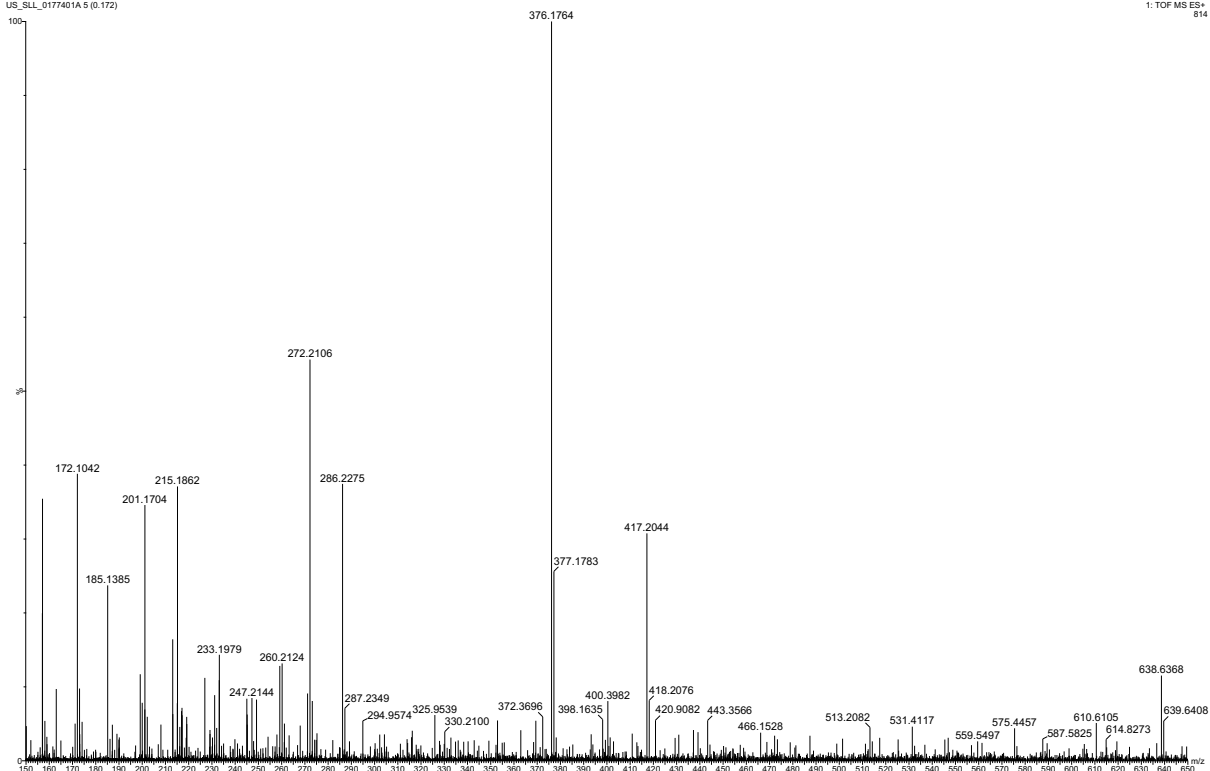


52

US_SLL_0177401
US_SLL_0177401A.5 (0.172)

ES-ToF

19-Dec-2017
1: TOF MS ES+
814



53, 54 Data not available