LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.184	481	484	496	rBV	40856	47470	2.61%	0.354%
2	5.272	496	499	503	rVB	27243	25428	1.40%	0.189%
3	5.589	550	553	571	rVB	807340	751343	41.33%	5.596%
4	6.589	720	723	733	rBV	494904	463904	25.52%	3.455%
5	6.731	742	747	750	rBV	1544130	1366539	75.18%	10.178%
6	6.954	781	785	791	rBB	458648	402219	22.13%	2.996%
7	7.107	807	811	815	rBV	1322526	1203680	66.22%	8.965%
8	7.519	876	881	884	rBV	1100811	1047630	57.63%	7.803%
9	8.236	999	1003	1013	rBV	484717	453900	24.97%	3.381%
10	9.307	1181	1185	1188	rBV	1867571	1643067	90.39%	12.238%
11	9.701	1246	1252	1257	rBV	103607	103444	5.69%	0.770%
12	9.901	1283	1286	1290	rBV	26849	21886	1.20%	0.163%
13	9.989	1298	1301	1310	rVB	435216	425669	23.42%	3.170%
14	10.401	1369	1371	1373	rVB	38958	26236	1.44%	0.195%
15	10.789	1433	1437	1440	rBV	1023036	969114	53.31%	7.218%
16	10.871	1448	1451	1454	rBV	29102	25672	1.41%	0.191%
17	10.901	1454	1456	1462	rVB	74358	65255	3.59%	0.486%
18	10.954	1462	1465	1467	rBV	152142	119748	6.59%	0.892%
19	10.989	1467	1471	1474	rVV2	148847	185954	10.23%	1.385%
20	11.024	1474	1477	1479	rVV2	161453	162632	8.95%	1.211%
21	11.048	1479	1481	1483	rVV	89724	68668	3.78%	0.511%
22	11.089	1483	1488	1489	rVV2	68721	85318	4.69%	0.635%
23	11.101	1489	1490	1493	rVV	64066	52601	2.89%	0.392%
24	11.136	1493	1496	1499	rVV3	142289	153968	8.47%	1.147%
25	11.171	1499	1502	1504	rVV	158878	130132	7.16%	0.969%
26	11.213	1507	1509	1514	rVB2	95386	75178	4.14%	0.560%
27	11.324	1525	1528	1531	rBV2	16512	19288	1.06%	0.144%
28	11.483	1552	1555	1562	rBV	435004	395410	21.75%	2.945%
29	13.071	1820	1825	1828	rBV	1967156	1817741	100.00%	13.539%
30	13.948	1971	1974	1980	rBV	75543	76194	4.19%	0.568%
31	14.142	2003	2007	2013	rBV	566332	576931	31.74%	4.297%
32	15.677	2263	2268	2278	rVB	340271	463903	25.52%	3.455%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-35

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

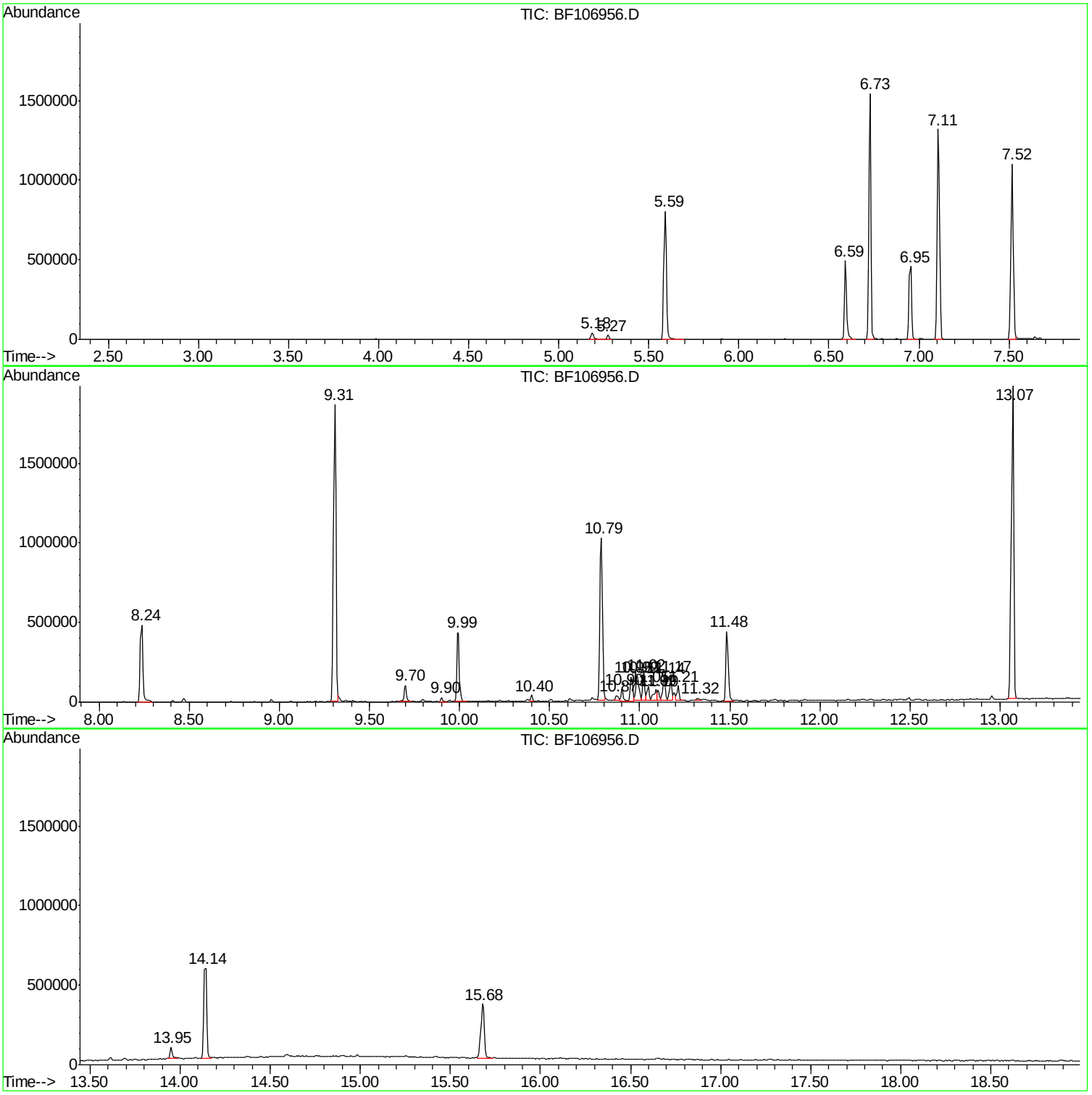
Sum of corrected areas: 13426122

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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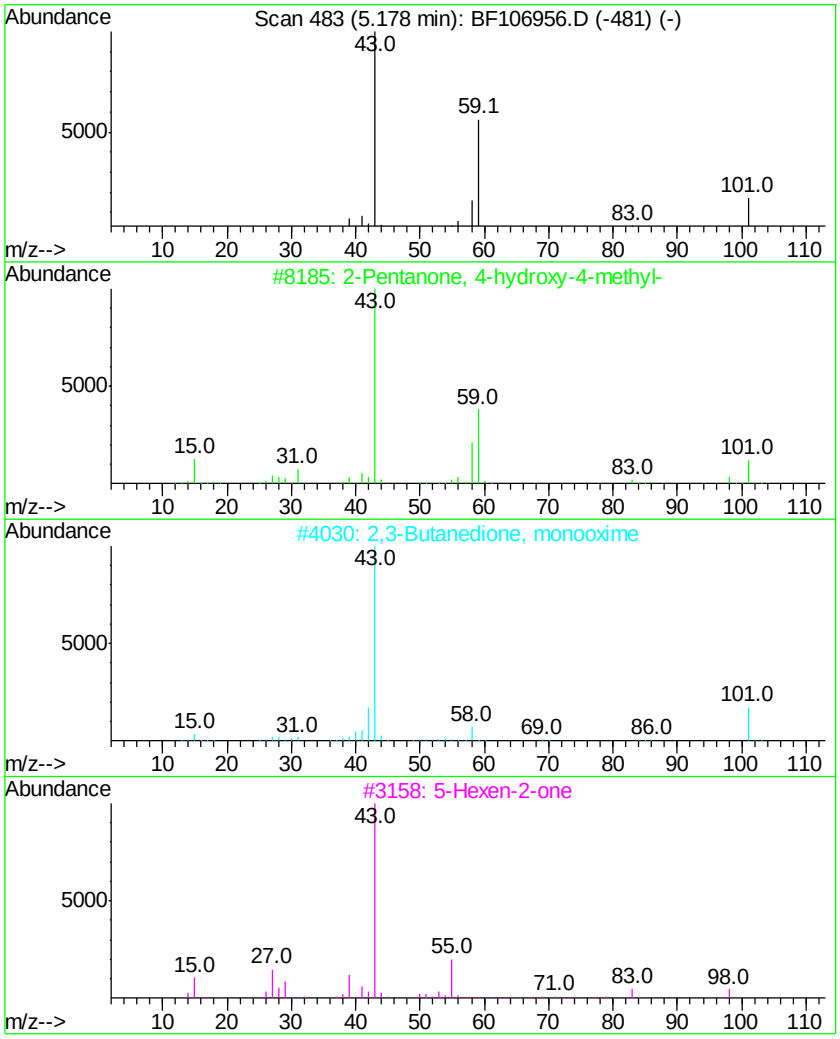
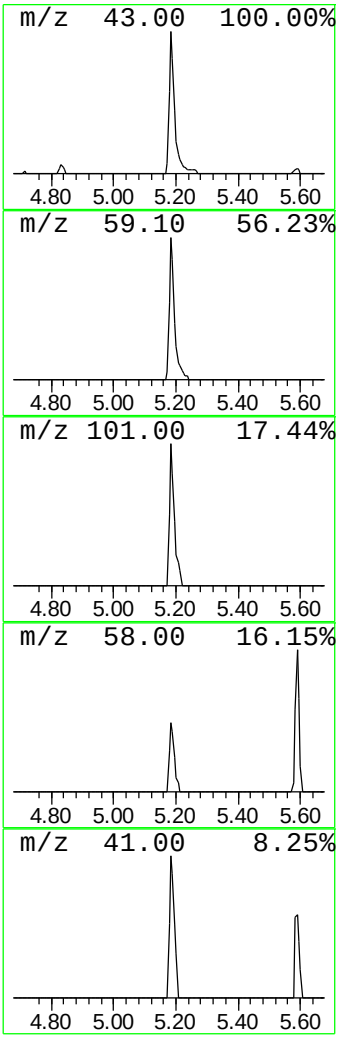
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	2.36 ng	47470	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

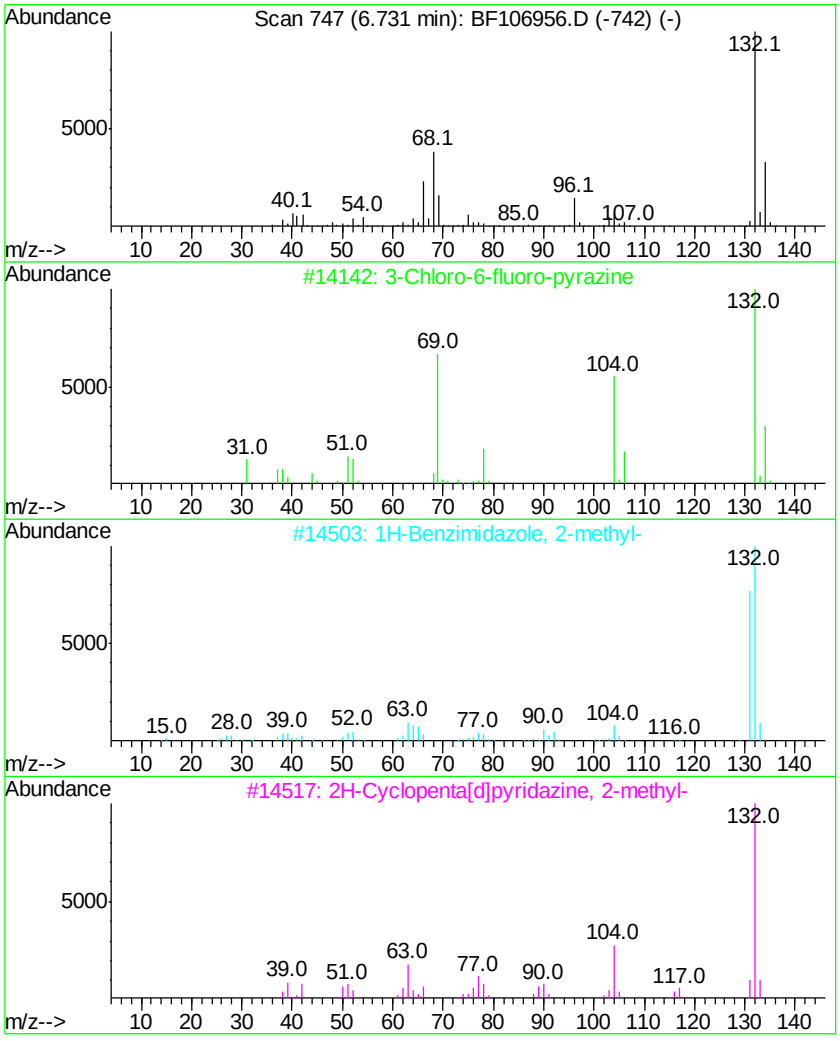
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

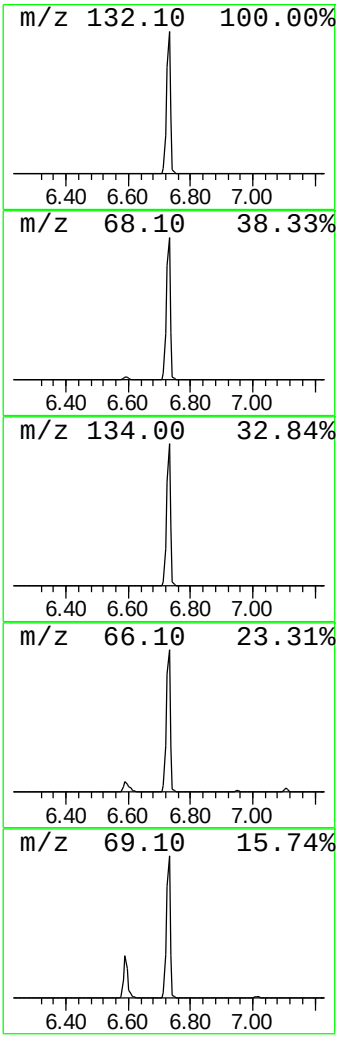
****

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	67.95 ng	1366540	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

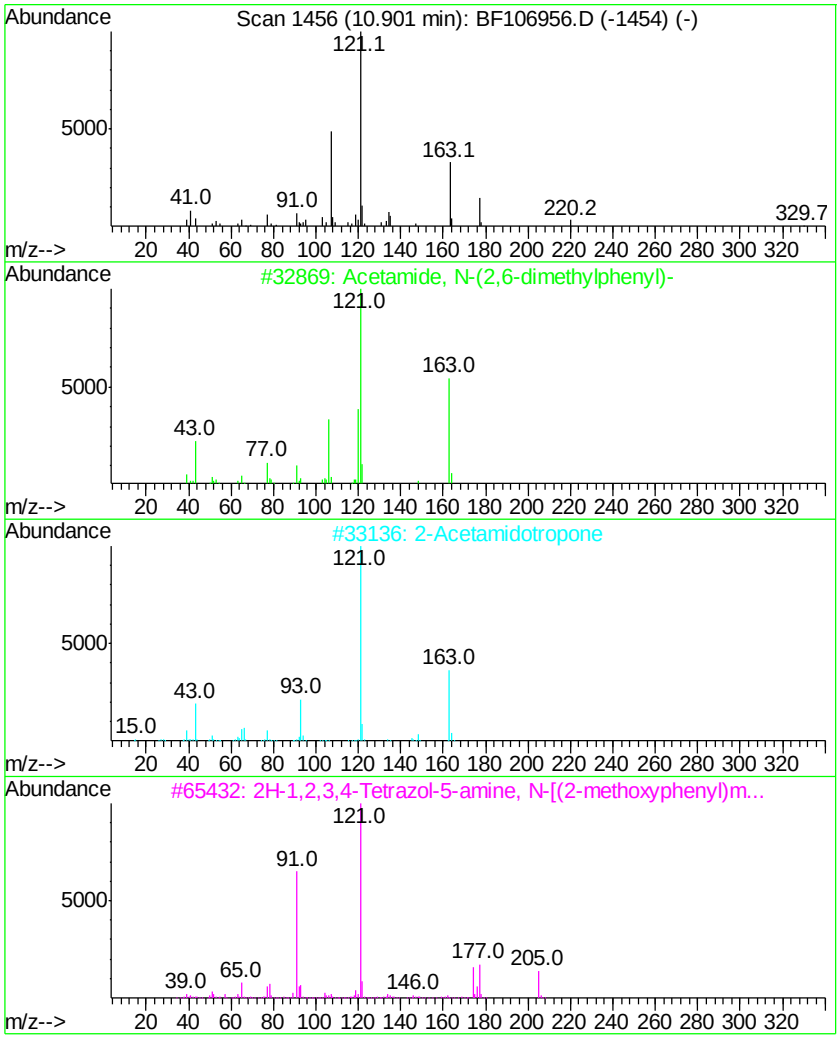
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

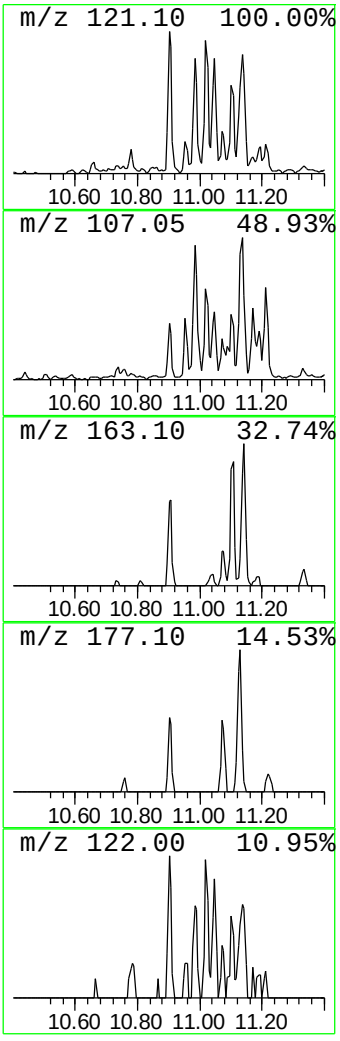
****

Peak Number 4 Acetamide, N-(2,6-dimethylp... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	3.30 ng	65255	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2,6-dimethylphenyl)-	163	C10H13NO	002198-53-0	52
2	2-Acetamidotropone	163	C9H9NO2	006422-12-4	49
3	2H-1,2,3,4-Tetrazol-5-amine, N-[...	205	C9H11N5O	1000337-56-1	47
4	1,2,4-Oxadiazol-5-amine, 3-[4-(c...	328	C15H16N6O3	1000351-08-7	47
5	2-Propanone, 1-(4-methoxyphenyl)-	164	C10H12O2	000122-84-9	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

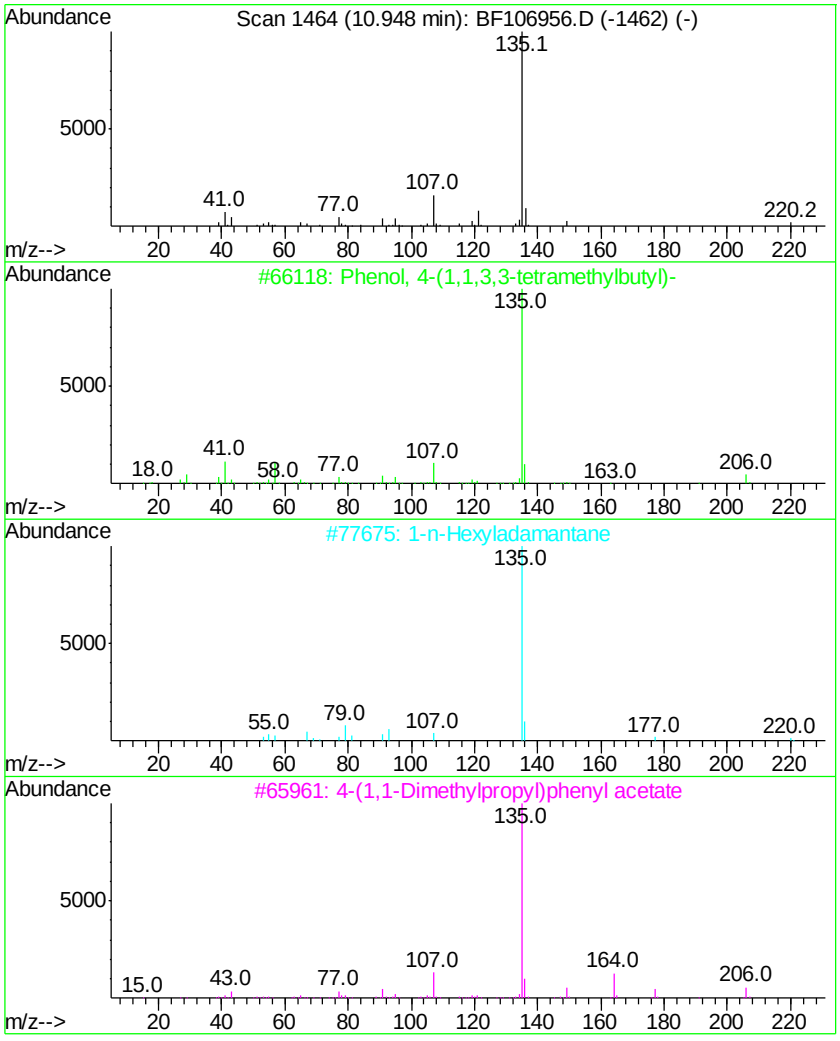
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

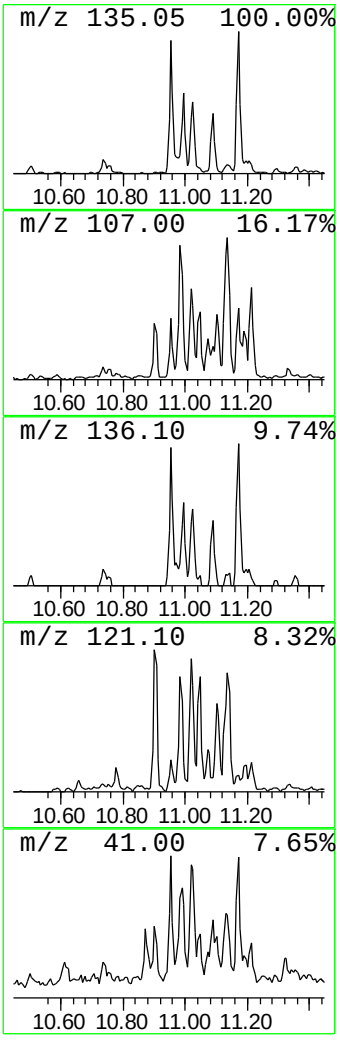
****

Peak Number 5 Phenol, 4-(1,1,3,3-tetramet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.95	6.06 ng	119748	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
2	1-n-Hexyladamantane	220	C16H28	022458-75-9	64
3	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	64
4	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	64
5	Pentanoic acid, 5-hydroxy-, p-t-...	250	C15H22O3	166273-37-6	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

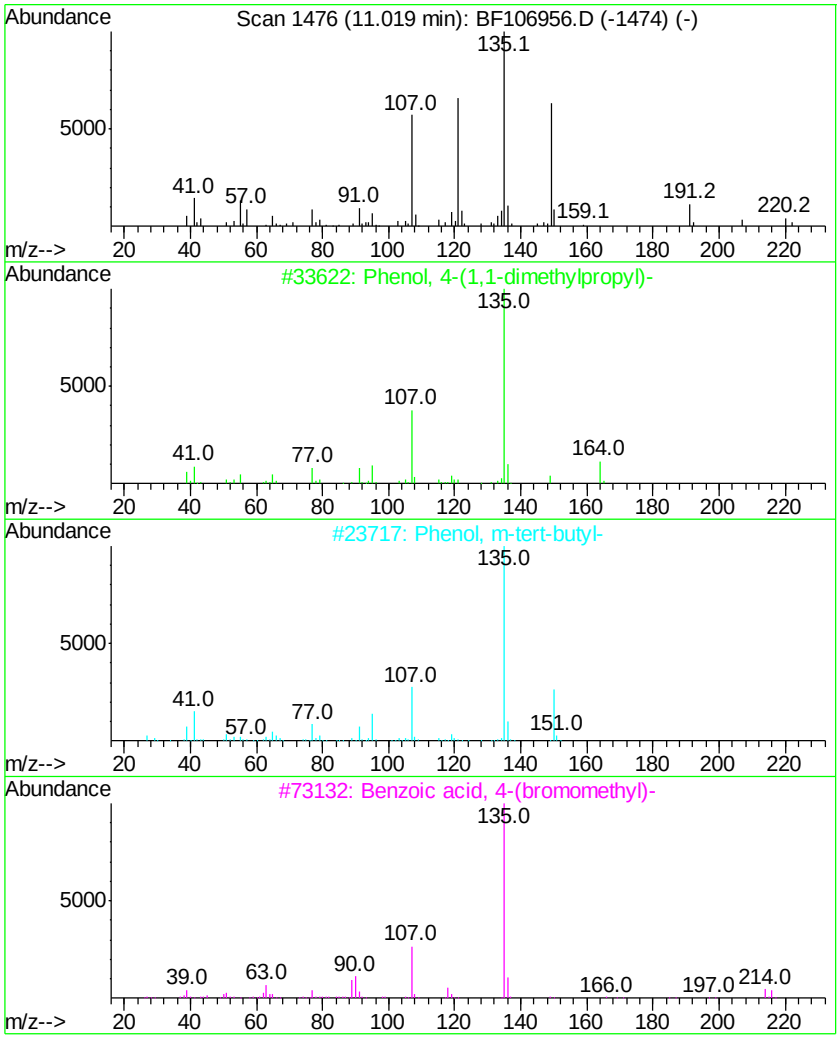
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

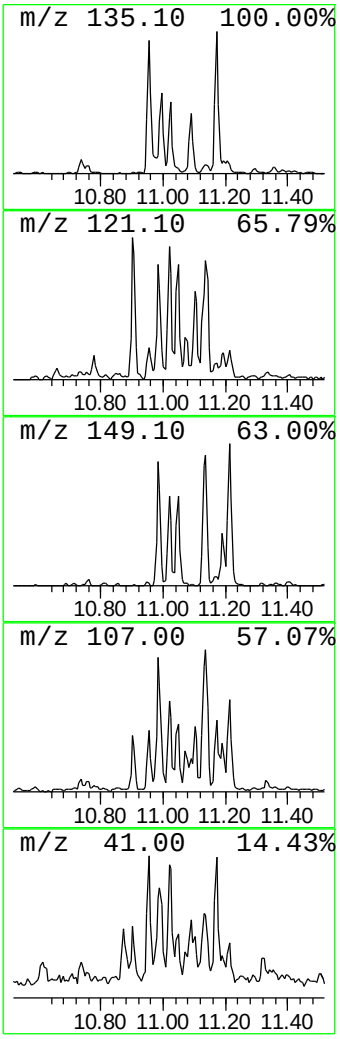
****

Peak Number 7 Phenol, 4-(1,1-dimethylprop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	8.23 ng	162632	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	53
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	52
3	Benzoic acid, 4-(bromomethyl)-	214	C8H7BrO2	006232-88-8	50
4	Hexestrol, O-heptafluorobutyryl-	466	C22H21F7O3	1000365-31-9	50
5	1-Adamantanecarboxamide, N,N-dim...	207	C13H21NO	001502-00-7	50





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Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

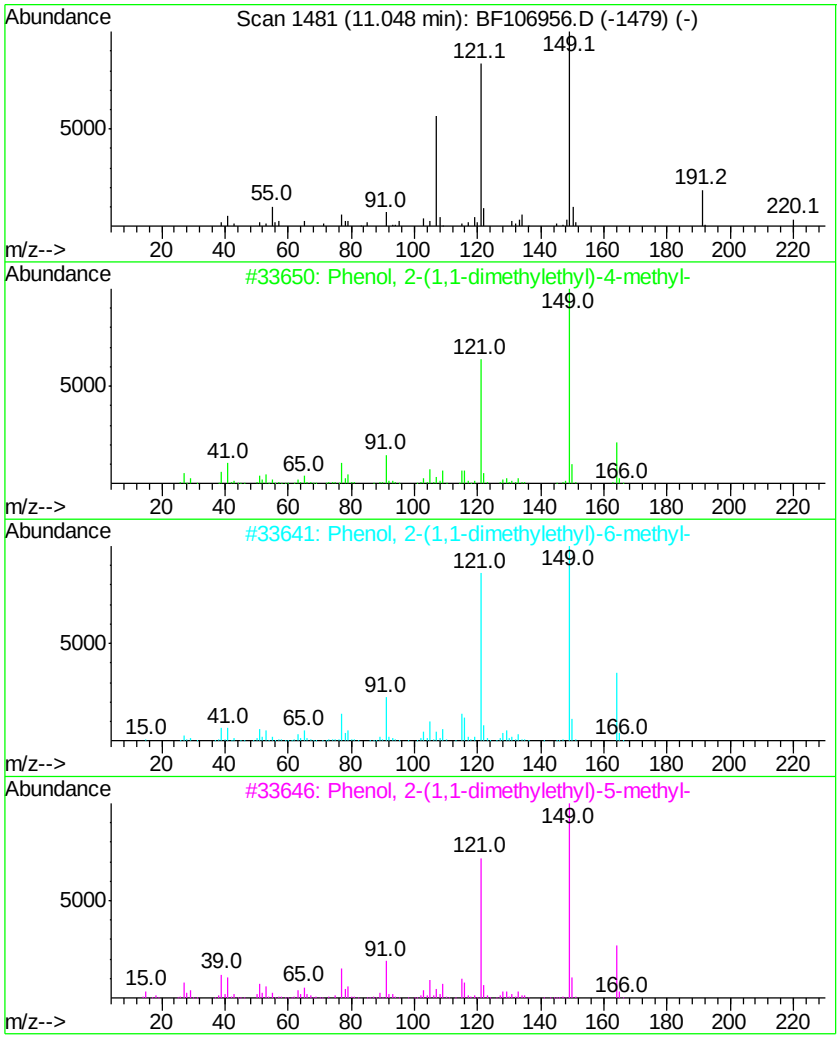
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

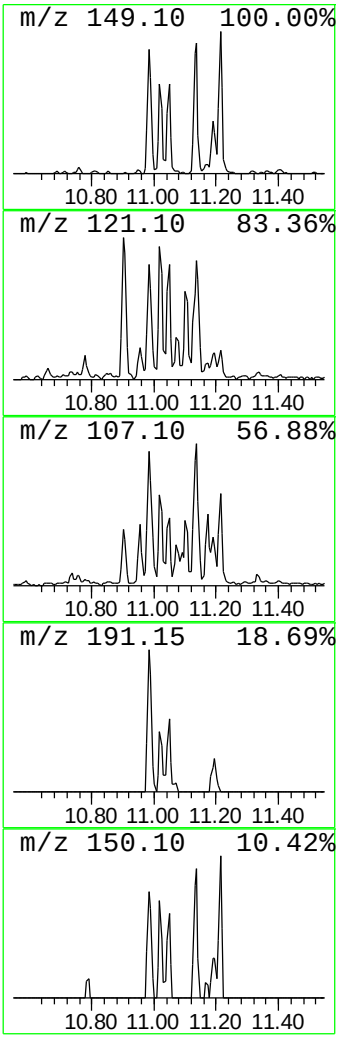
****

Peak Number 8 Phenol, 2-(1,1-dimethylethy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	3.47 ng	68668	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2-(1,1-dimethylethyl)-4-...	164	C11H16O	002409-55-4	59
2	Phenol, 2-(1,1-dimethylethyl)-6-...	164	C11H16O	002219-82-1	59
3	Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	53
4	6-Amino-1-methylpurine	149	C6H7N5	005142-22-3	35
5	7-Methylthieno[3,2-b]pyridine	149	C8H7NS	013362-83-9	35





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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

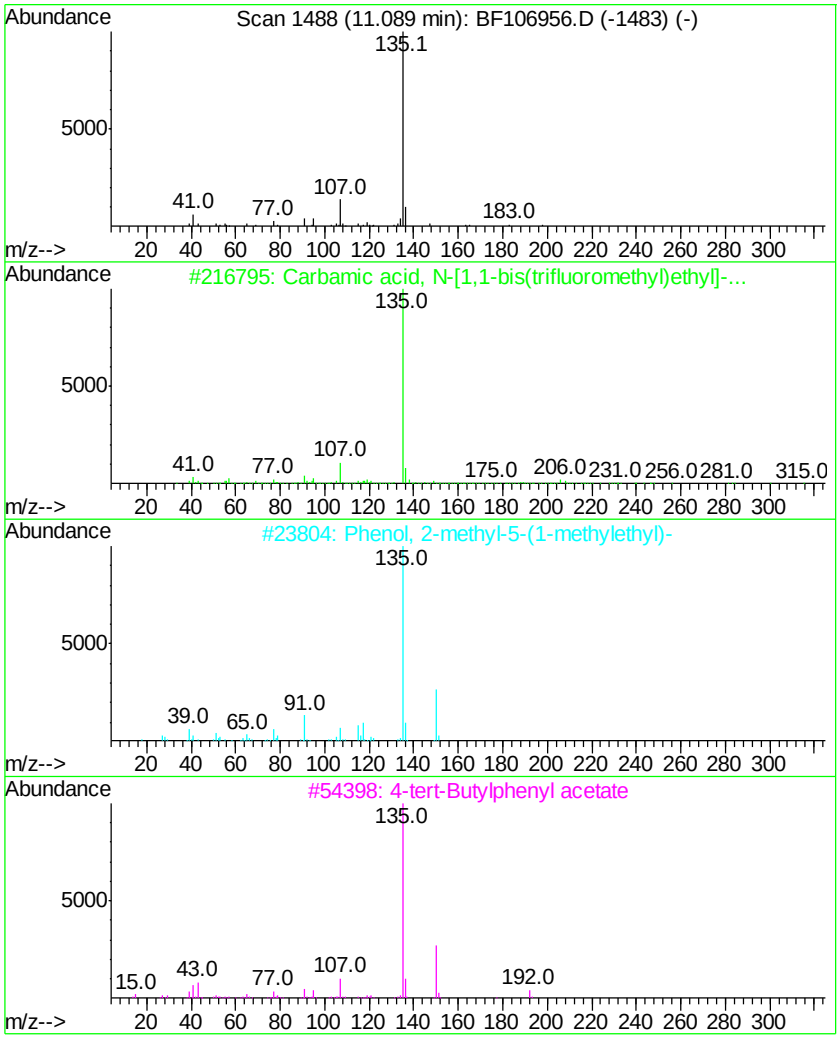
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

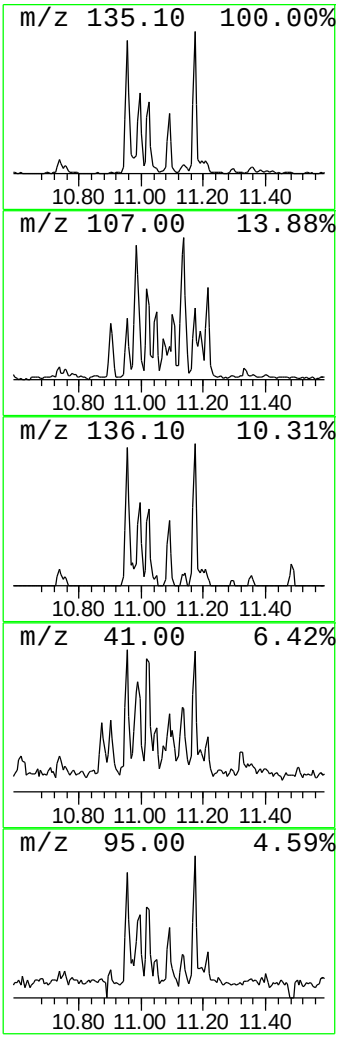
****

Peak Number 9 Carbamic acid, N-[1,1-bis(t... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	4.32 ng	85318	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	72
2	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	000499-75-2	72
3	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	72
4	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	72
5	Hexestrol, O-heptafluorobutyryl-	466	C22H21F7O3	1000365-31-9	64





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Misc :
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Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

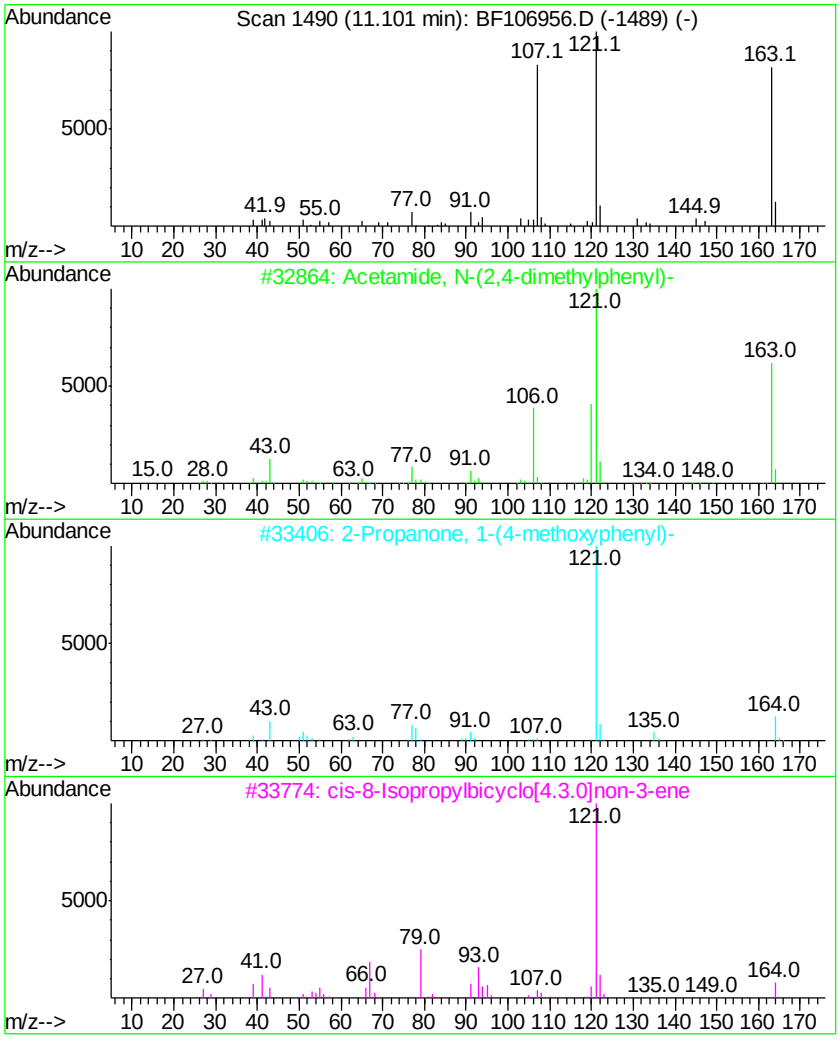
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

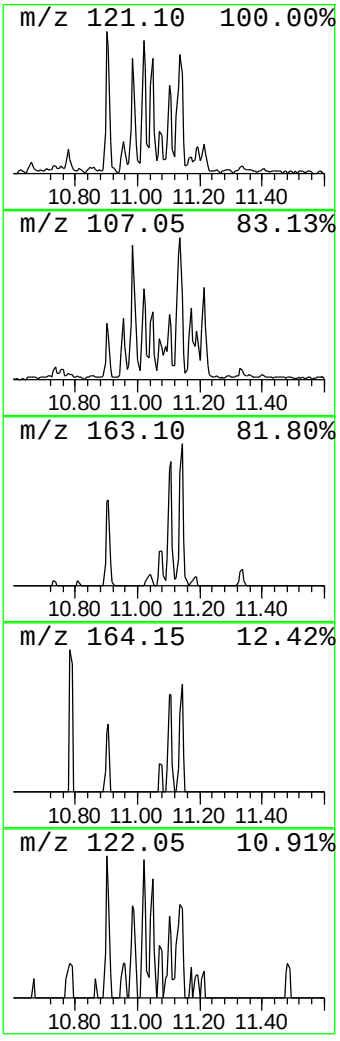
****

Peak Number 10 Acetamide, N-(2,4-dimethylp... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.66 ng	52601	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2,4-dimethylphenyl)-	163	C10H13NO	002050-43-3	52
2	2-Propanone, 1-(4-methoxyphenyl)-	164	C10H12O2	000122-84-9	25
3	cis-8-Isopropylbicyclo[4.3.0]non...	164	C12H20	1000145-85-1	22
4	Benzenamine, 2,4-dimethyl-	121	C8H11N	000095-68-1	14
5	Fenipentol	164	C11H16O	000583-03-9	14





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Instrument : BNA_F
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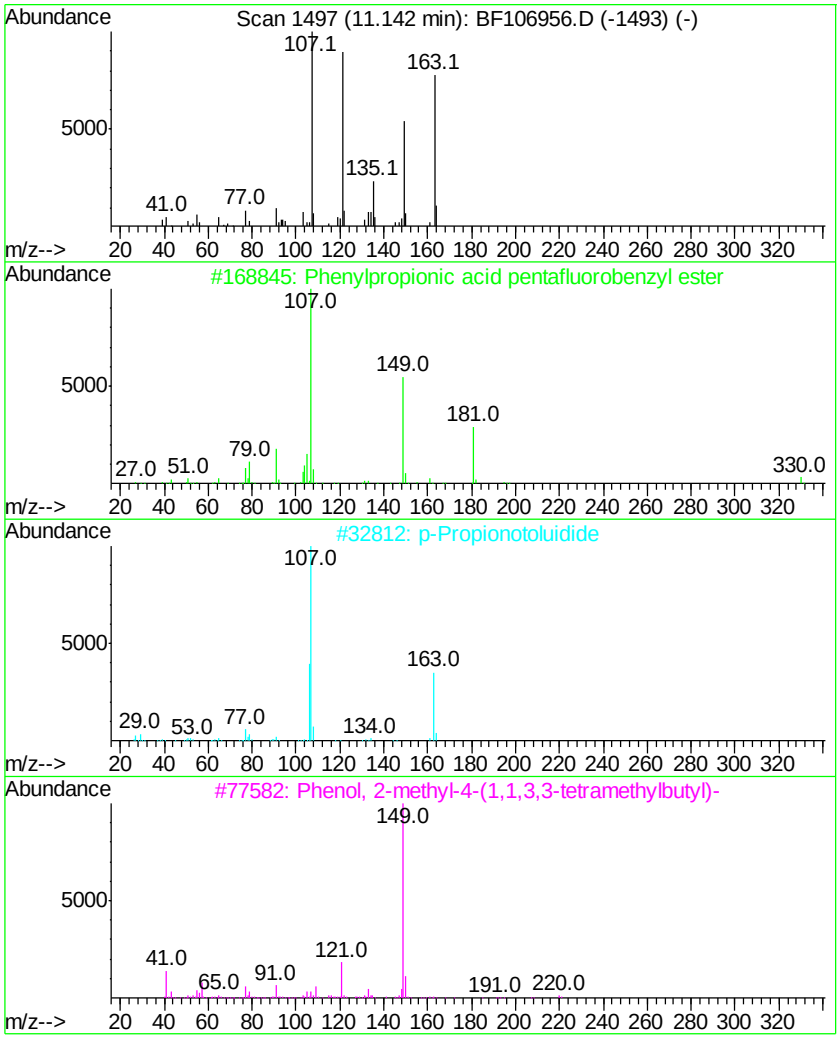
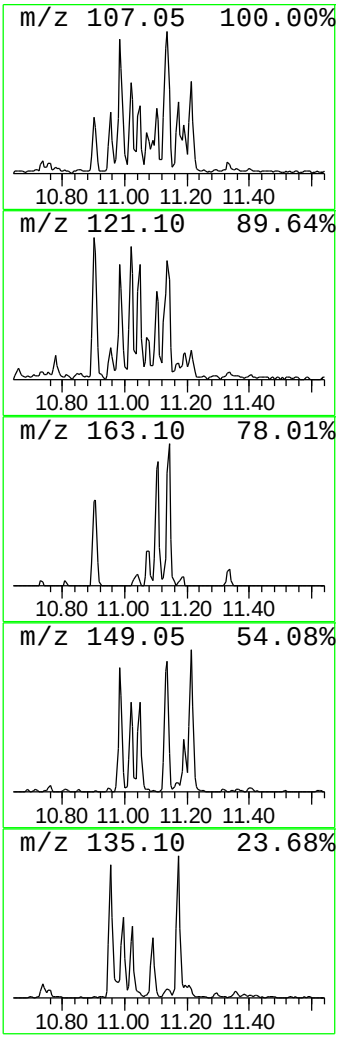
****

Peak Number 11 unknown11.14 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	7.79 ng	153968	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenylpropionic acid pentafluoro...	330	C16H11F5O2	062434-95-1	43
2	p-Propionotoluidide	163	C10H13NO	002759-55-9	38
3	Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	38
4	3',4'-(Methylenedioxy)acetophenone	164	C9H8O3	003162-29-6	35
5	3-Methyl-1-adamantaneacetic acid	208	C13H20O2	014202-13-2	35





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Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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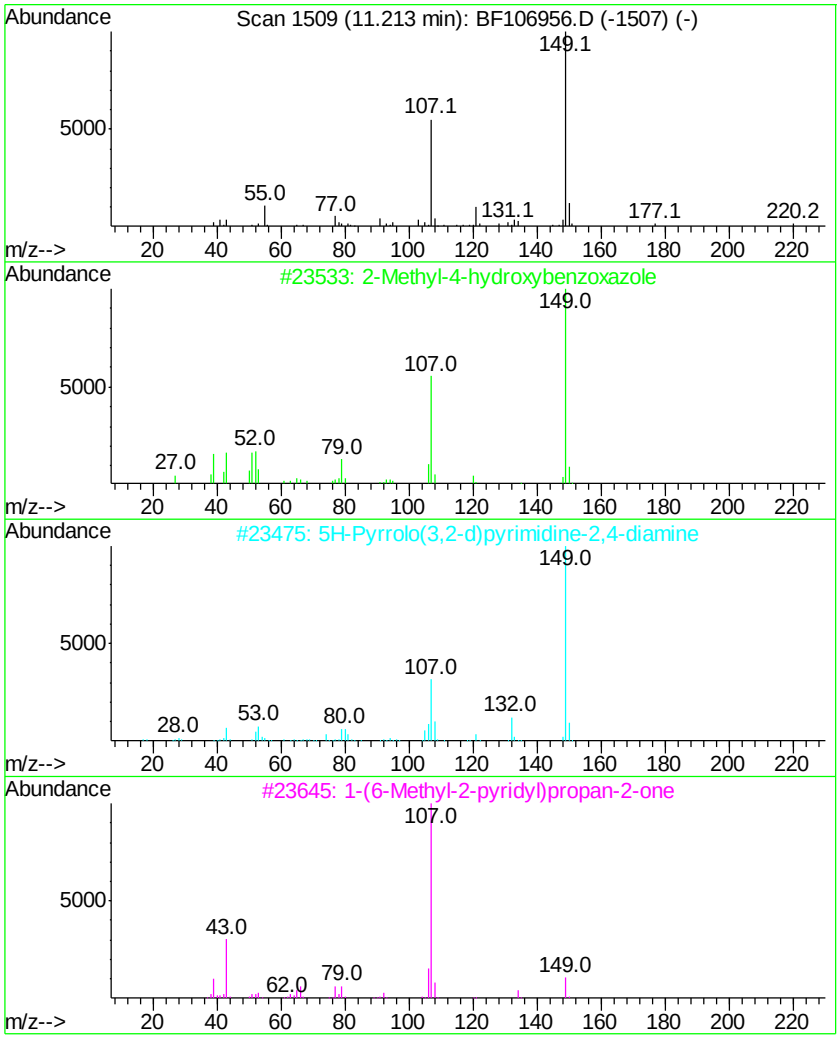
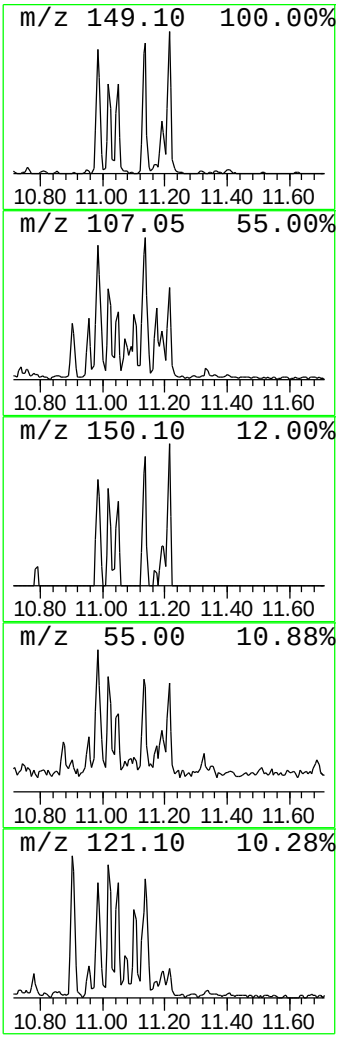
Peak Number 13 2-Methyl-4-hydroxybenzoxazole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.21	3.80 ng	75178	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	72
2	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	72
3	1-(6-Methyl-2-pyridyl)propan-2-one	149	C9H11NO	065702-08-1	72
4	1,3-Cyclopentadiene, 5,5-dimethy...	178	C13H22	1000163-88-0	59
5	Acetamide, 2-(4-cyclohexylphenox...	324	C20H24N2O2	1000263-95-6	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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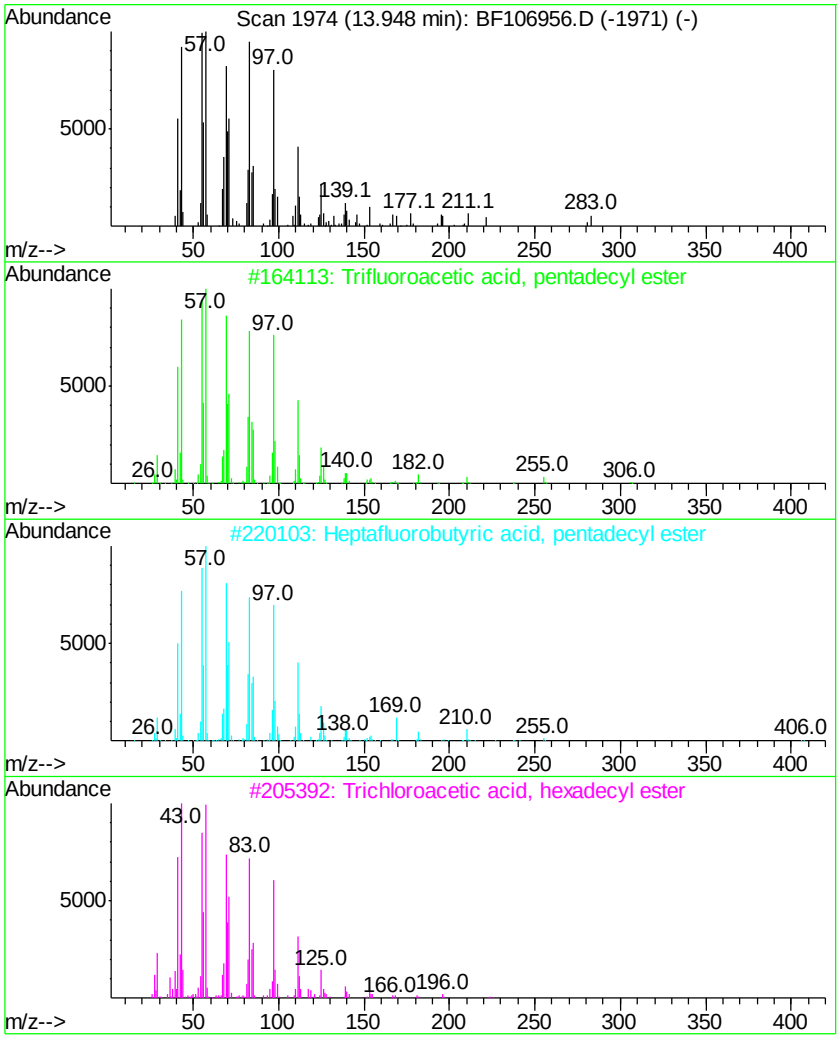
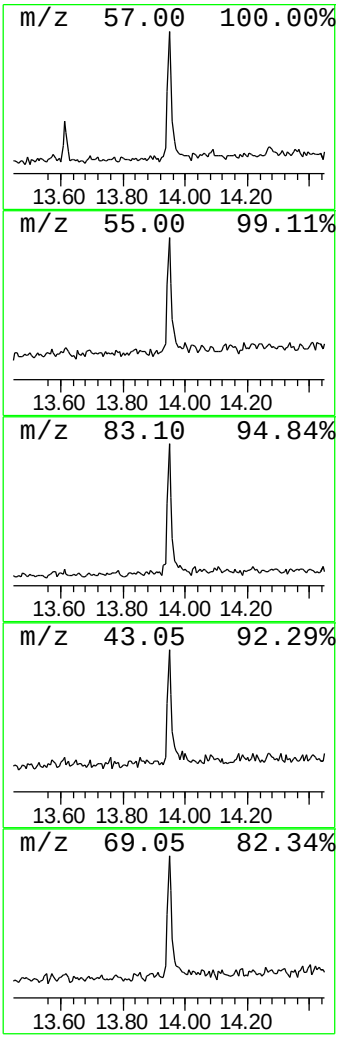
Peak Number 14 Trifluoroacetic acid, penta... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	2.64 ng	76194	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4	1-Nonadecene	266	C19H38	018435-45-5	94
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062818\
Data File : BF106956.D
Acq On : 29 Jun 2018 7:35
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.18	2.4	ng	47470	1	6.95	402219	20.0
unknown6.73	6.73	68.0	ng	1366540	1	6.95	402219	20.0
Acetamide, N-(2,6...	10.90	3.3	ng	65255	4	11.48	395410	20.0
Phenol, 4-(1,1,3,...	10.95	6.1	ng	119748	4	11.48	395410	20.0
Phenol, 4-(1,1-di...	11.02	8.2	ng	162632	4	11.48	395410	20.0
Phenol, 2-(1,1-di...	11.05	3.5	ng	68668	4	11.48	395410	20.0
Carbamic acid, N-...	11.09	4.3	ng	85318	4	11.48	395410	20.0
Acetamide, N-(2,4...	11.10	2.7	ng	52601	4	11.48	395410	20.0
unknown11.14	11.14	7.8	ng	153968	4	11.48	395410	20.0
2-Methyl-4-hydrox...	11.21	3.8	ng	75178	4	11.48	395410	20.0
Trifluoroacetic a...	13.95	2.6	ng	76194	5	14.14	576931	20.0