LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 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	492	rBV	24718	26897	2.39%	0.340%
2	5.278	497	500	503	rBB	16015	14096	1.25%	0.178%
3	5.595	550	554	567	rBB	496983	443751	39.43%	5.602%
4	6.595	720	724	736	rBV	280956	277044	24.61%	3.498%
5	6.731	743	747	750	rBV	905146	825539	73.34%	10.422%
6	6.954	782	785	788	rBV	301323	235505	20.92%	2.973%
7	7.113	807	812	815	rBV	799528	717794	63.77%	9.062%
8	7.519	876	881	884	rBV	621365	624170	55.45%	7.880%
9	8.236	999	1003	1019	rBV	314074	264847	23.53%	3.344%
10	9.313	1181	1186	1189	rBV	1046146	977760	86.87%	12.344%
11	9.701	1249	1252	1256	rVB	69166	56327	5.00%	0.711%
12	9.901	1282	1286	1291	rBV	14334	13197	1.17%	0.167%
13	9.995	1298	1302	1309	rVB	299207	246421	21.89%	3.111%
14	10.401	1369	1371	1374	rVB	19997	16784	1.49%	0.212%
15	10.789	1433	1437	1443	rVB	638765	578241	51.37%	7.300%
16	10.877	1449	1452	1454	rBV	18136	13347	1.19%	0.168%
17	10.907	1454	1457	1460	rVB	47531	34013	3.02%	0.429%
18	10.960	1463	1466	1468	rBV	82851	70101	6.23%	0.885%
19	10.989	1468	1471	1474	rVV2	93958	107338	9.54%	1.355%
20	11.024	1474	1477	1479	rVV2	109636	94705	8.41%	1.196%
21	11.048	1479	1481	1484	rVV	56283	45586	4.05%	0.576%
22	11.077	1484	1486	1487	rVV	21383	19123	1.70%	0.241%
23	11.095	1487	1489	1490	rVV	34700	33865	3.01%	0.428%
24	11.107	1490	1491	1493	rVV	38540	22929	2.04%	0.289%
25	11.136	1493	1496	1500	rVV3	83264	93067	8.27%	1.175%
26	11.172	1500	1502	1505	rVV	80191	77333	6.87%	0.976%
27	11.219	1508	1510	1513	rVB2	49210	39650	3.52%	0.501%
28	11.489	1552	1556	1564	rVB	275663	234438	20.83%	2.960%
29	13.071	1821	1825	1829	rBV	1103921	1125556	100.00%	14.210%
30	13.948	1971	1974	1979	rBV	49269	51351	4.56%	0.648%
31	14.142	2003	2007	2014	rBV	339870	318286	28.28%	4.018%
32	15.677	2263	2268	2275	rVB	170472	222012	19.72%	2.803%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 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

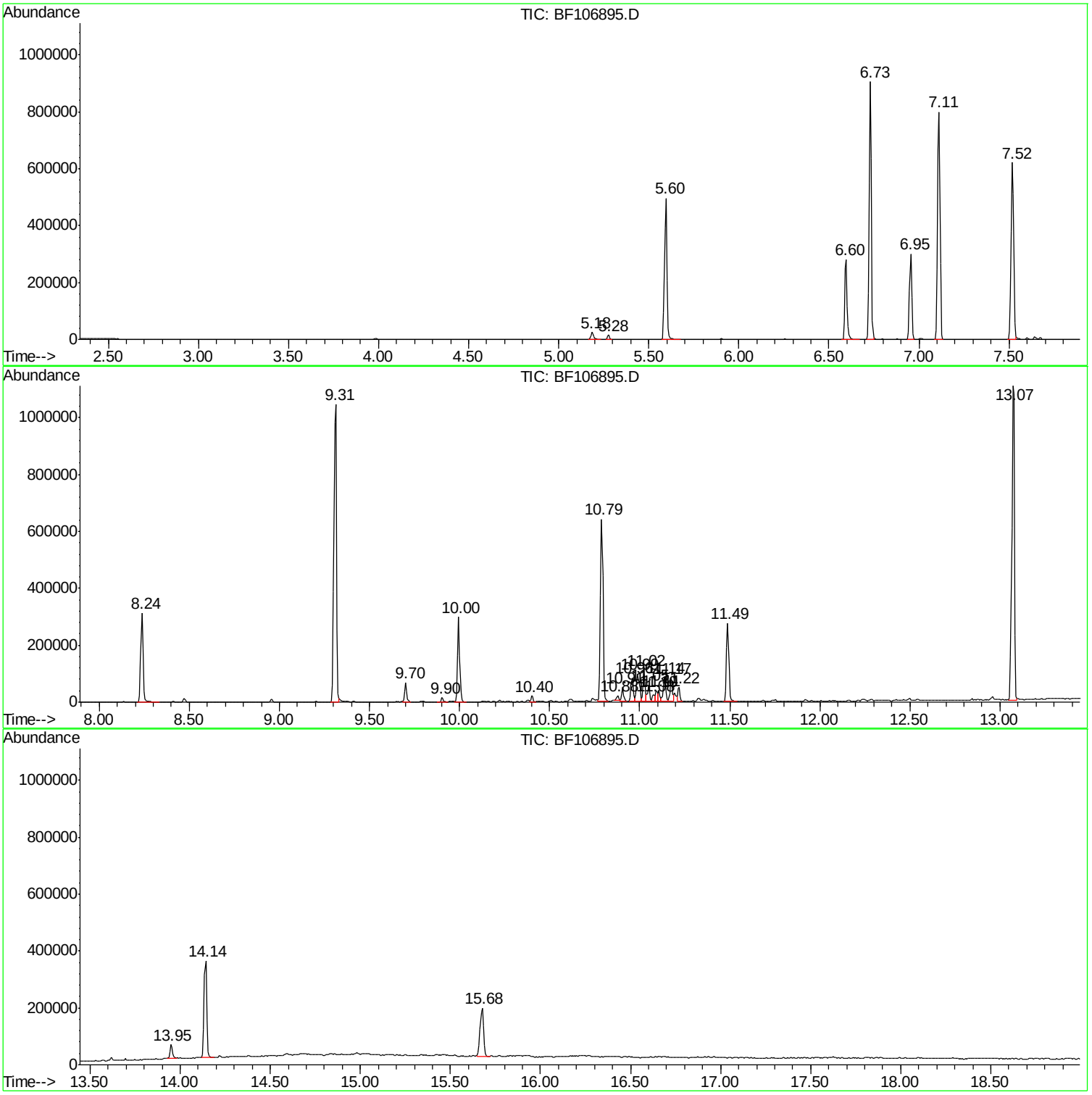
Sum of corrected areas: 7921073

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
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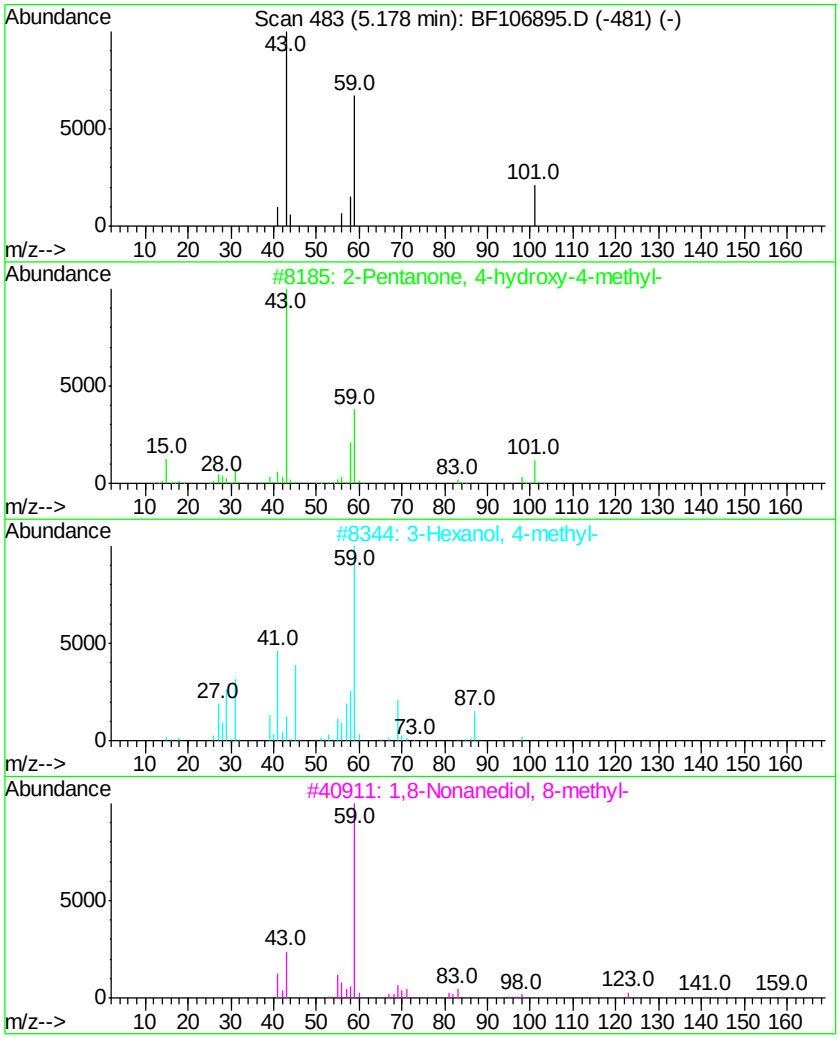
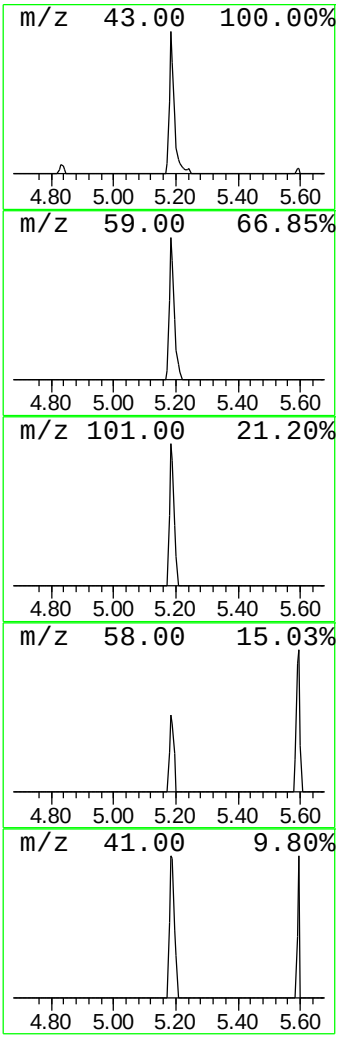
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	2.28 ng	26897	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	78
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9
4	3-Pentanol	88	C5H12O	000584-02-1	9
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 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

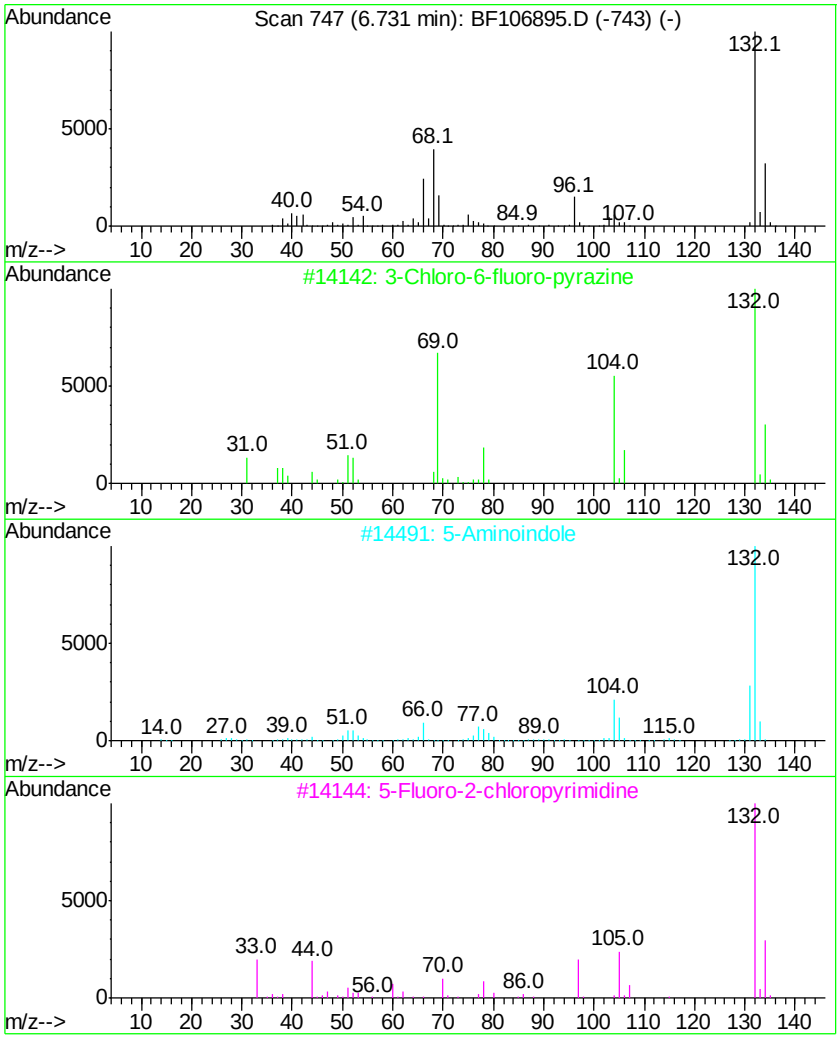
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

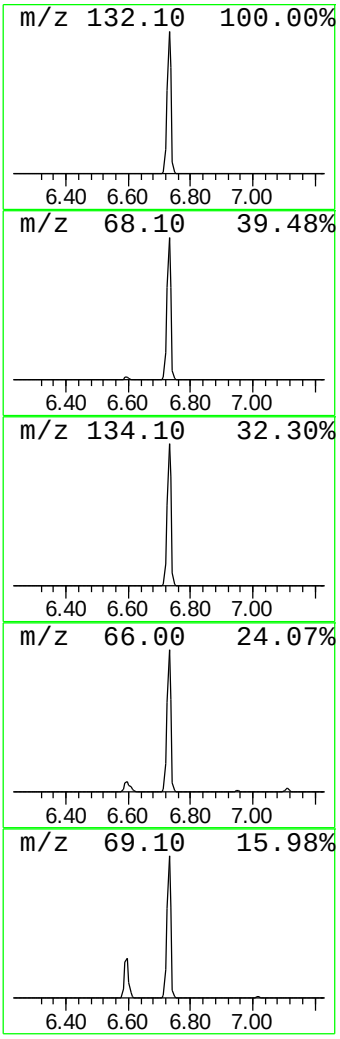
****

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	70.11 ng	825539	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	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 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

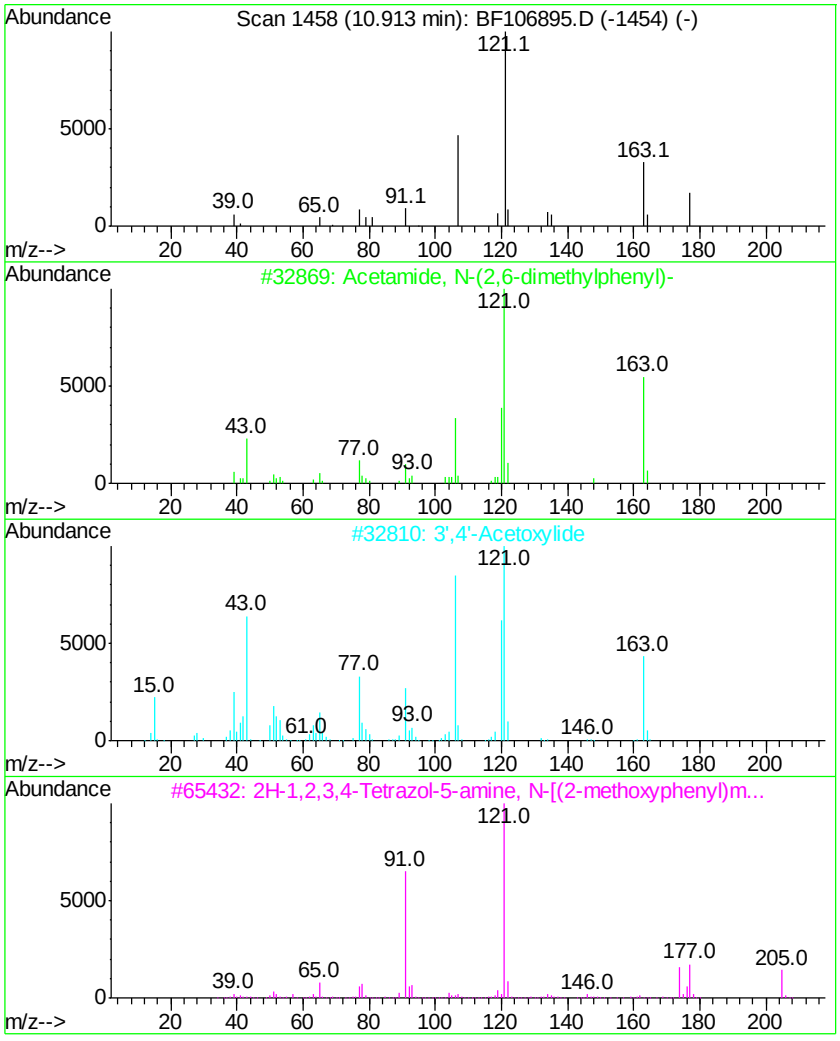
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

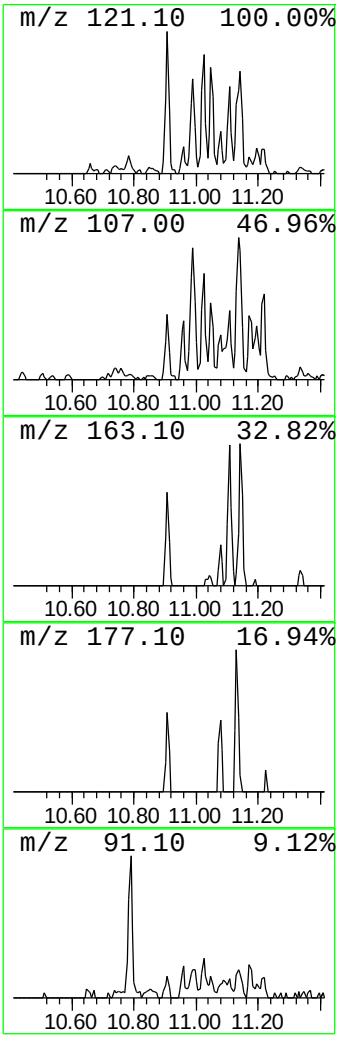
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	2.90 ng	34013	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(2,6-dimethylphenyl)-	163	C10H13NO	002198-53-0	52
2	3',4'-Acetoxylide	163	C10H13NO	002198-54-1	50
3	2H-1,2,3,4-Tetrazol-5-amine, N-[...	205	C9H11N5O	1000337-56-1	47
4	2-Acetamidotropone	163	C9H9NO2	006422-12-4	47
5	Benzene, 1-(2-bromoethyl)-4-meth...	214	C9H11BrO	014425-64-0	43





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 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

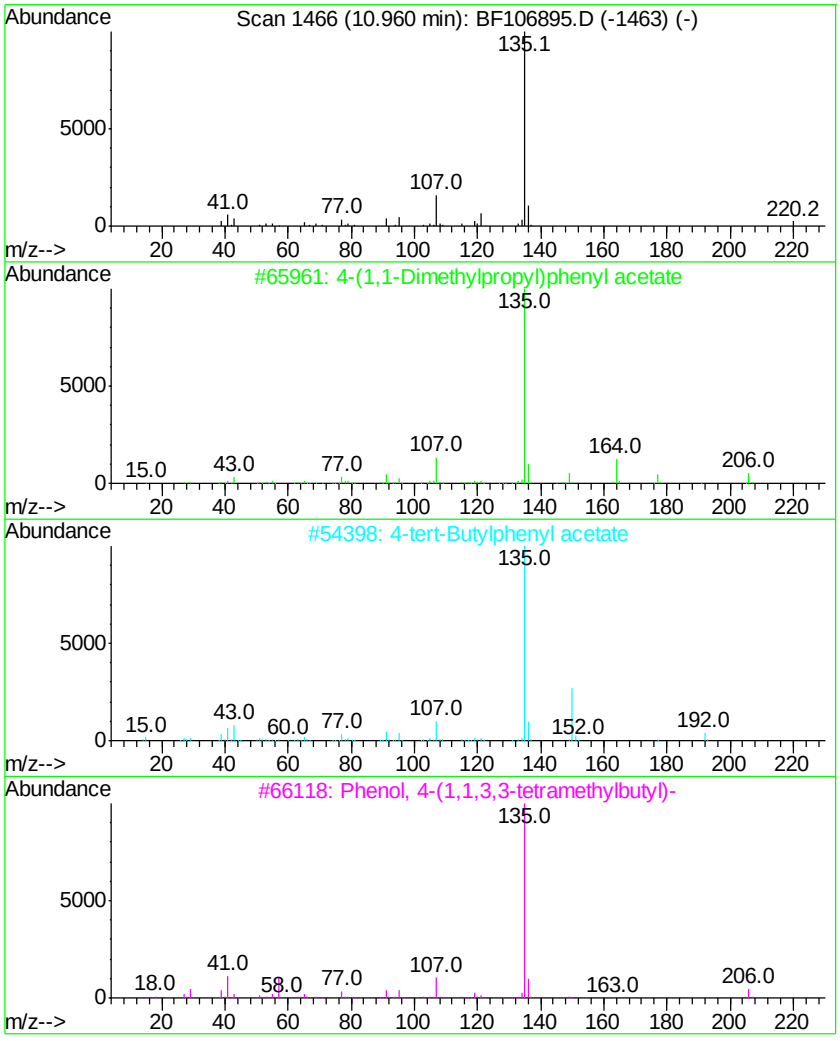
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

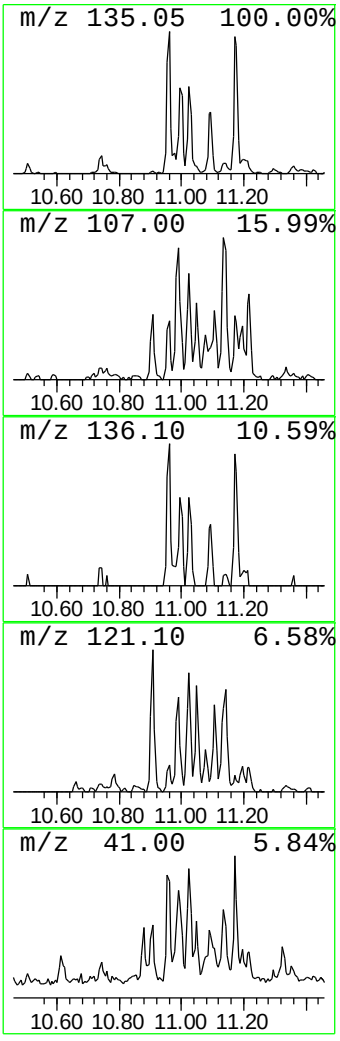
****

Peak Number 5 4-(1,1-Dimethylpropyl)pheny... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	5.98 ng	70101	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(1,1-Dimethylpropyl)phenyl ace...	206	C13H18O2	1000373-45-3	78
2	4-tert-Butylphenyl acetate	192	C12H16O2	003056-64-2	78
3	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	78
4	Hexestrol	270	C18H22O2	000084-16-2	72
5	1-Adamantanecarboxylic acid, 3,4...	324	C17H18Cl2O2	1000307-66-4	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 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

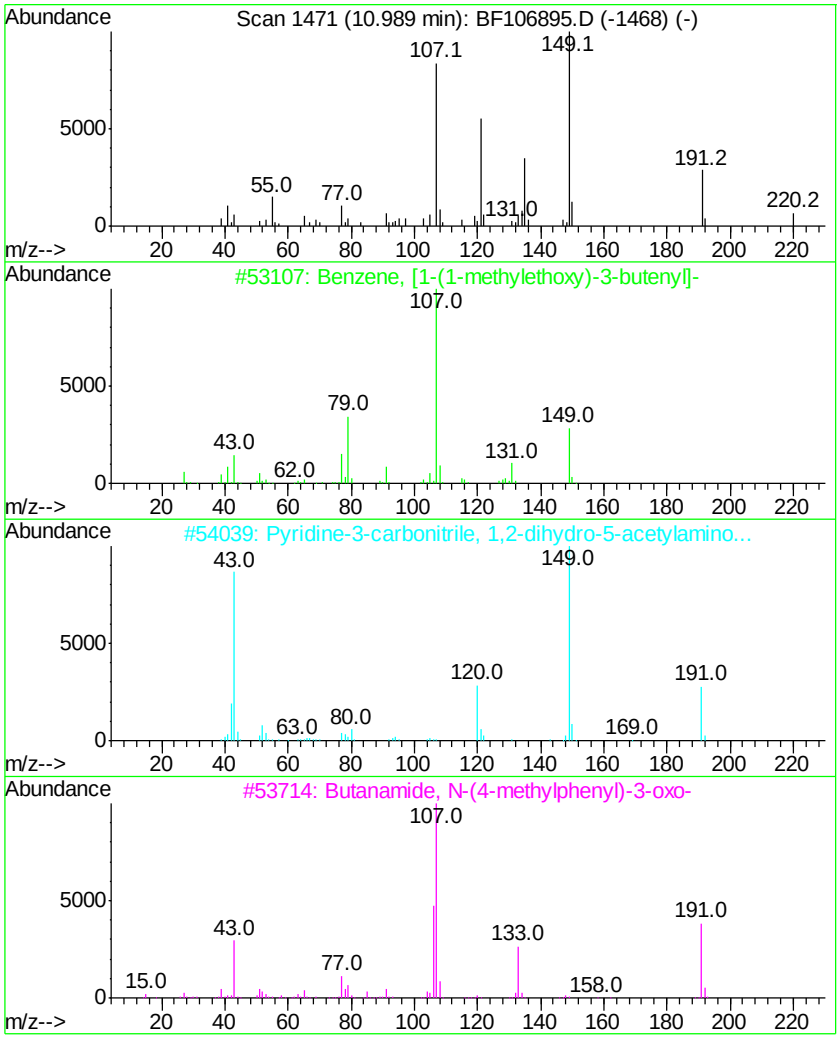
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

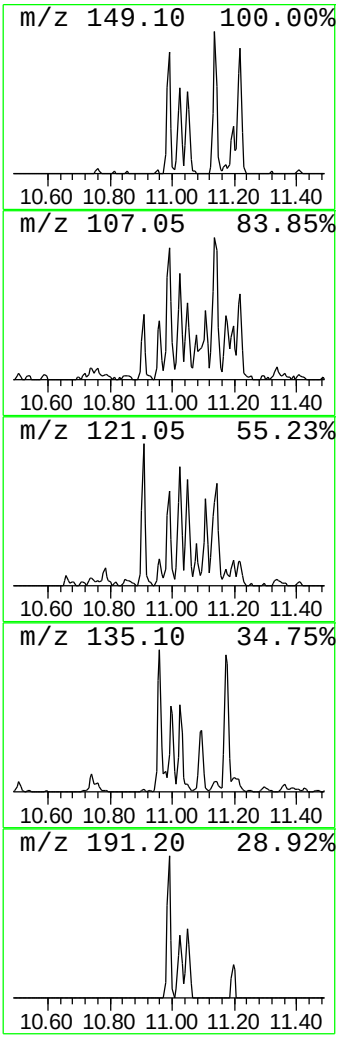
****

Peak Number 6 Benzene, [1-(1-methylethoxy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.99	9.16 ng	107338	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, [1-(1-methylethoxy)-3-b...	190	C13H18O	098088-47-2	53
2	Pyridine-3-carbonitrile, 1,2-dih...	191	C9H9N3O2	220098-92-0	43
3	Butanamide, N-(4-methylphenyl)-3...	191	C11H13NO2	002415-85-2	38
4	Phthalic acid, dec-2-yl propyl e...	348	C21H32O4	1000356-93-7	35
5	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	35





Library Search Compound Report

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Misc :
ALS Vial : 32 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
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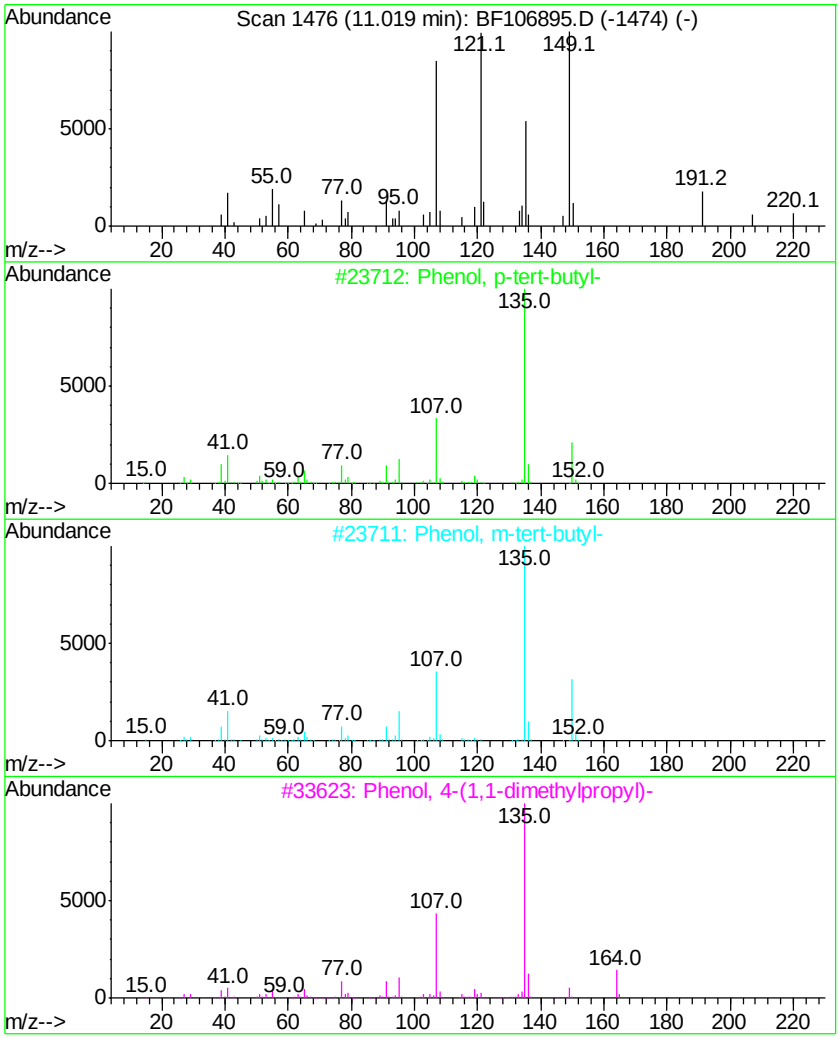
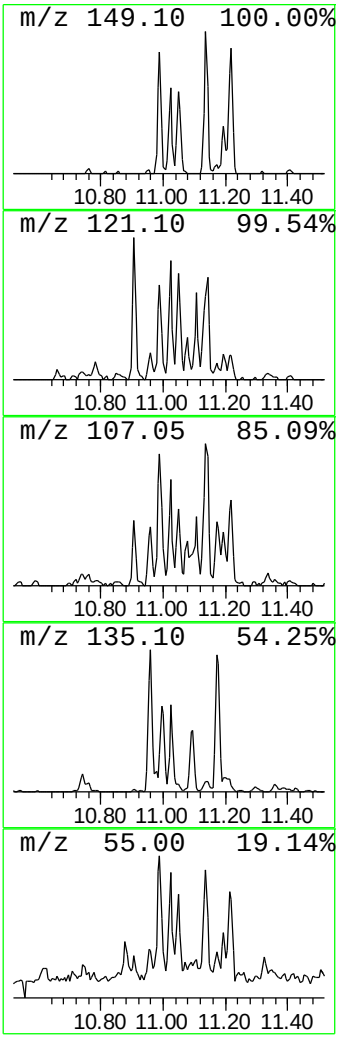
****

Peak Number 7 Phenol, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	8.08 ng	94705	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	60
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	47
3	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	47
4	Hexestrol, O-acetyl-	312	C20H24O3	1000374-87-8	47
5	p-Methoxybenzenepentanoic acid, ...	222	C12H14O4	004609-10-3	38





Library Search Compound Report

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Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
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Sample : J3693-06
Misc :
ALS Vial : 32 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
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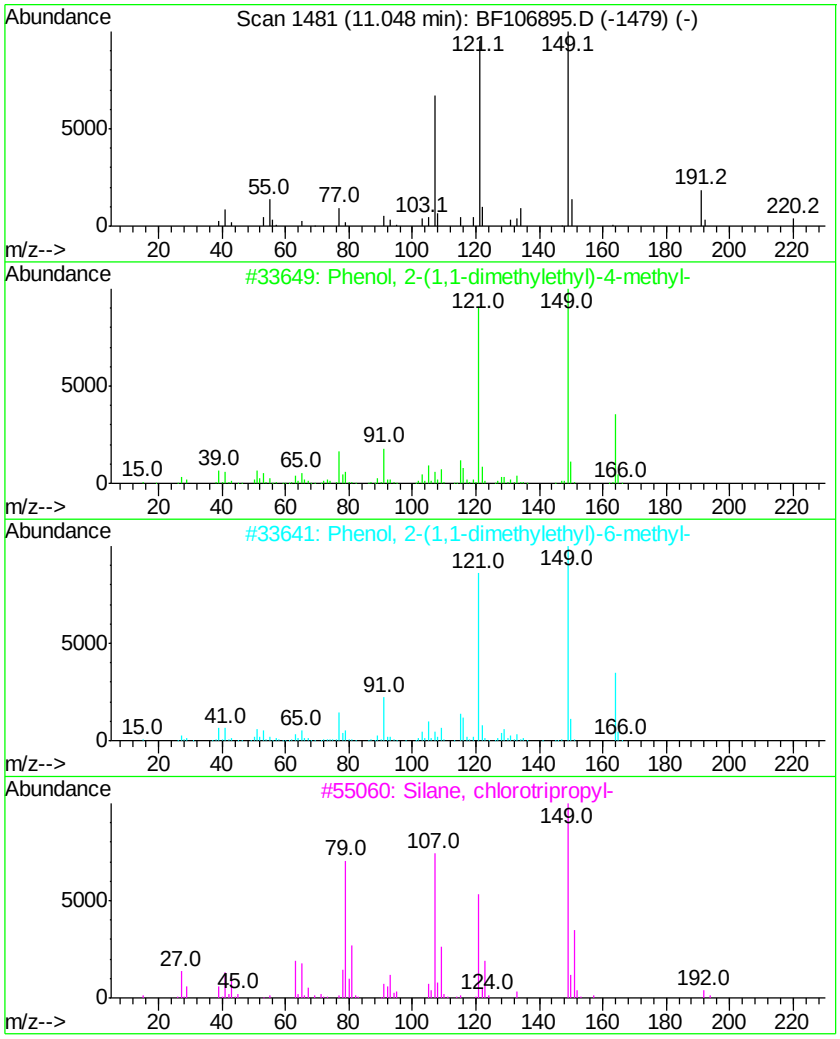
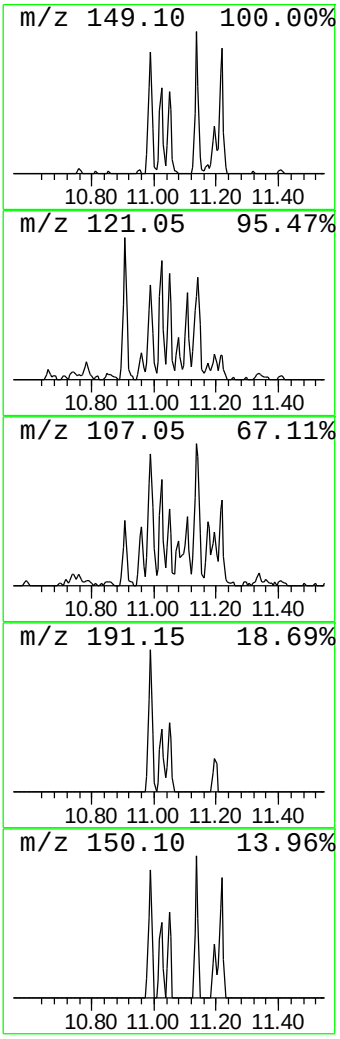
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	3.89 ng	45586	Phenanthrene-d10	11.49

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	Silane, chlorotripropyl-	192	C9H21ClSi	000995-25-5	47
4	Isoxazole, 4,5-dihydro-5-[(4-met...	191	C11H13NO2	1000362-14-0	30
5	Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	27





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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

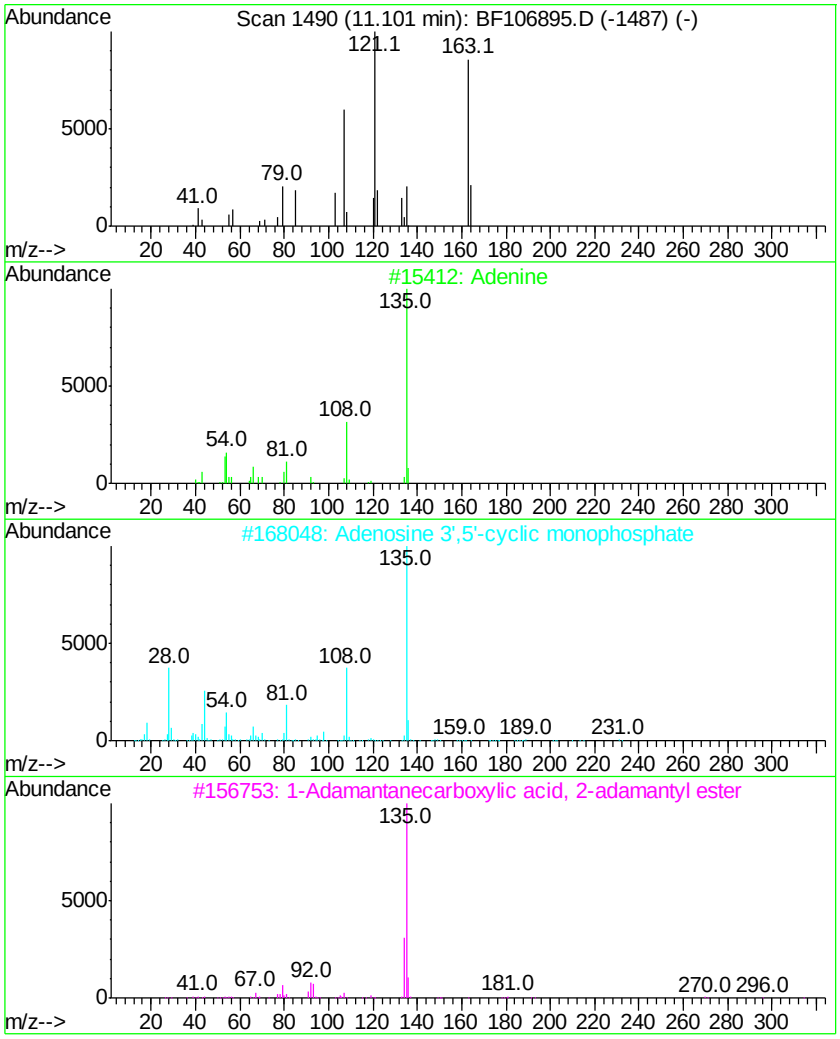
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

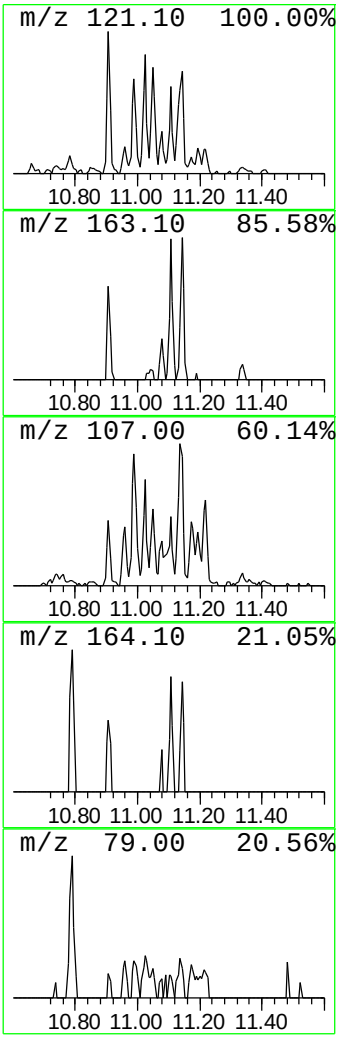
****

Peak Number 9 Adenine Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.89 ng	33865	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adenine	135	C5H5N5	000073-24-5	56
2	Adenosine 3',5'-cyclic monophosp...	329	C10H12N5O6P	000060-92-4	43
3	1-Adamantanecarboxylic acid, 2-a...	314	C21H30O2	1000282-94-3	40
4	Thioimidodicarbonic diamide	135	C2H5N3S2	000541-53-7	9
5	1,2-Benzenediol, O-(4-methoxyben...	338	C19H14O6	1000329-72-1	9





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ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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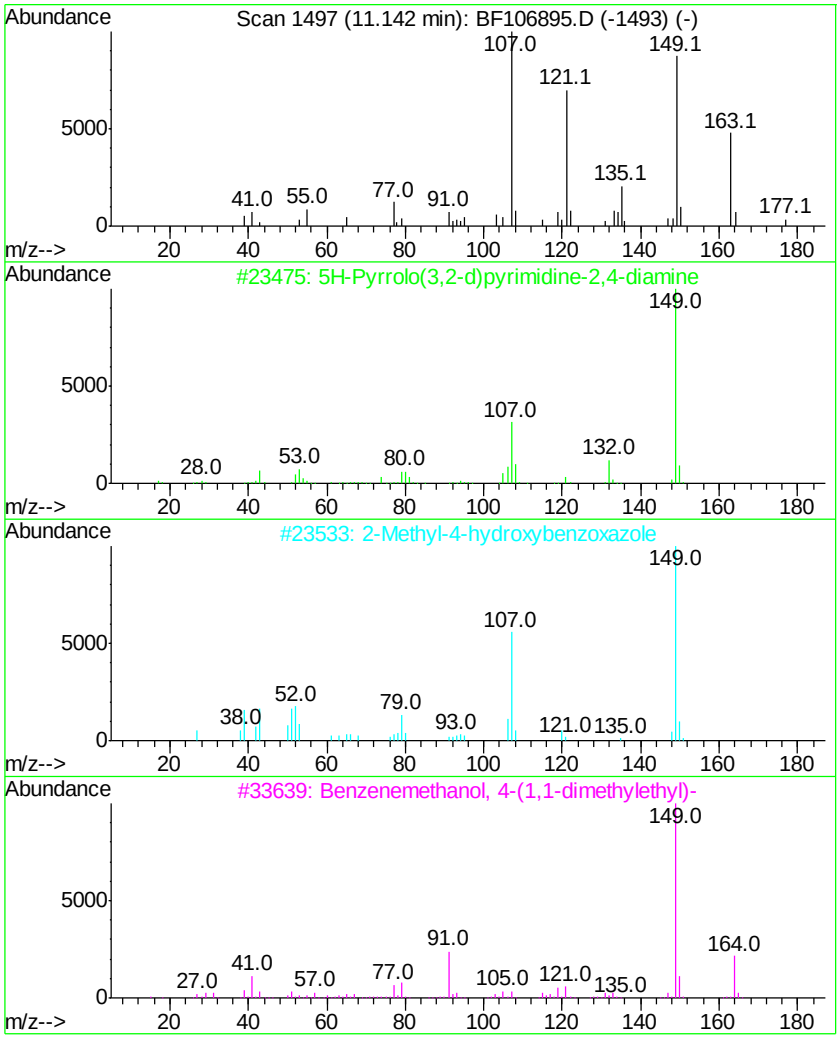
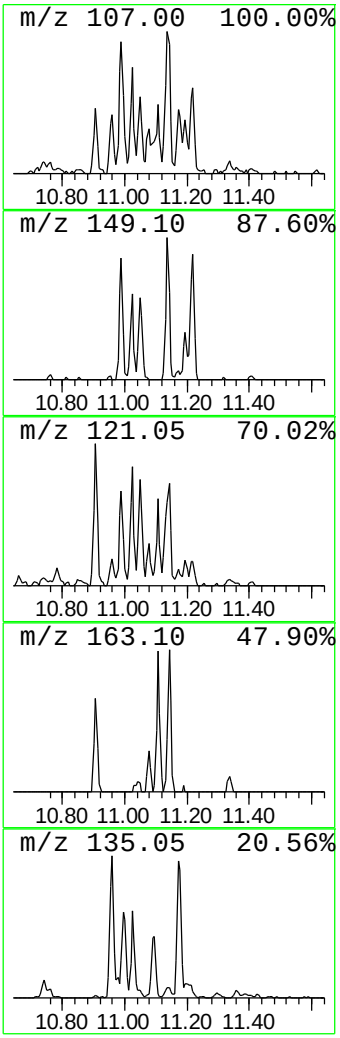
****

Peak Number 10 5H-Pyrrolo(3,2-d)pyrimidine... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.14	7.94 ng	93067	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	64
2	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	64
3	Benzenemethanol, 4-(1,1-dimethyl...	164	C11H16O	000877-65-6	38
4	2H-Indol-2-one, 1,3-dihydro-5-hy...	149	C8H7NO2	003416-18-0	35
5	Phthalic acid, ethyl tridec-2-yn...	372	C23H32O4	1000315-43-5	35





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 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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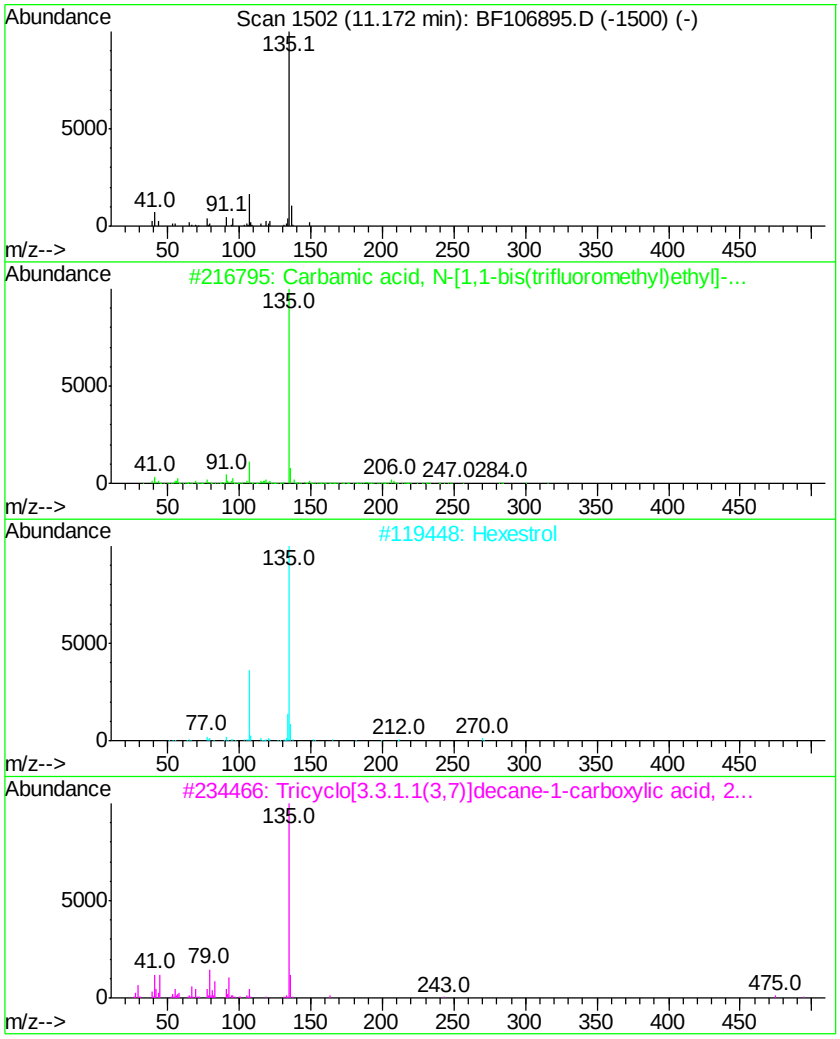
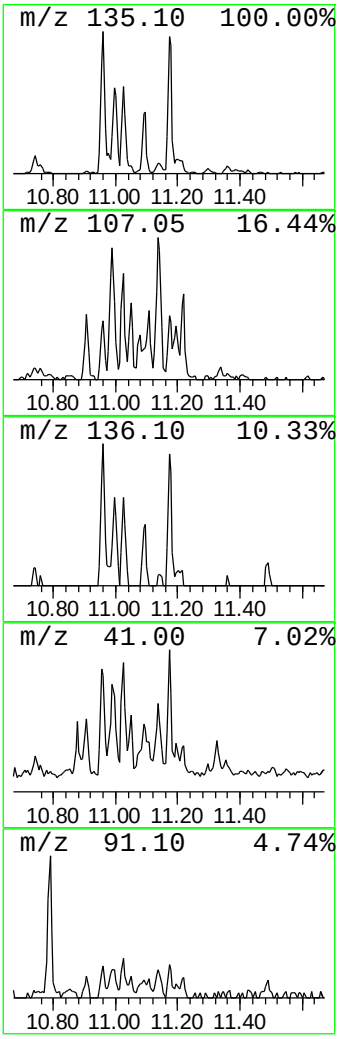
Peak Number 11 Carbamic acid, N-[1,1-bis(t... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	6.60 ng	77333	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6NO2	296242-69-8	78
2	Hexestrol	270	C18H22O2	000084-16-2	56
3	Tricyclo[3.3.1.1(3,7)]decane-1-c...	494	C18H18F12O2	1000141-65-1	50
4	1,3-Benzenediol, o-(2-furoyl)-o'...	338	C19H14O6	1000330-77-5	50
5	1-Adamantanecarboxylic acid chlo...	198	C11H15ClO	002094-72-6	45





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Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-35

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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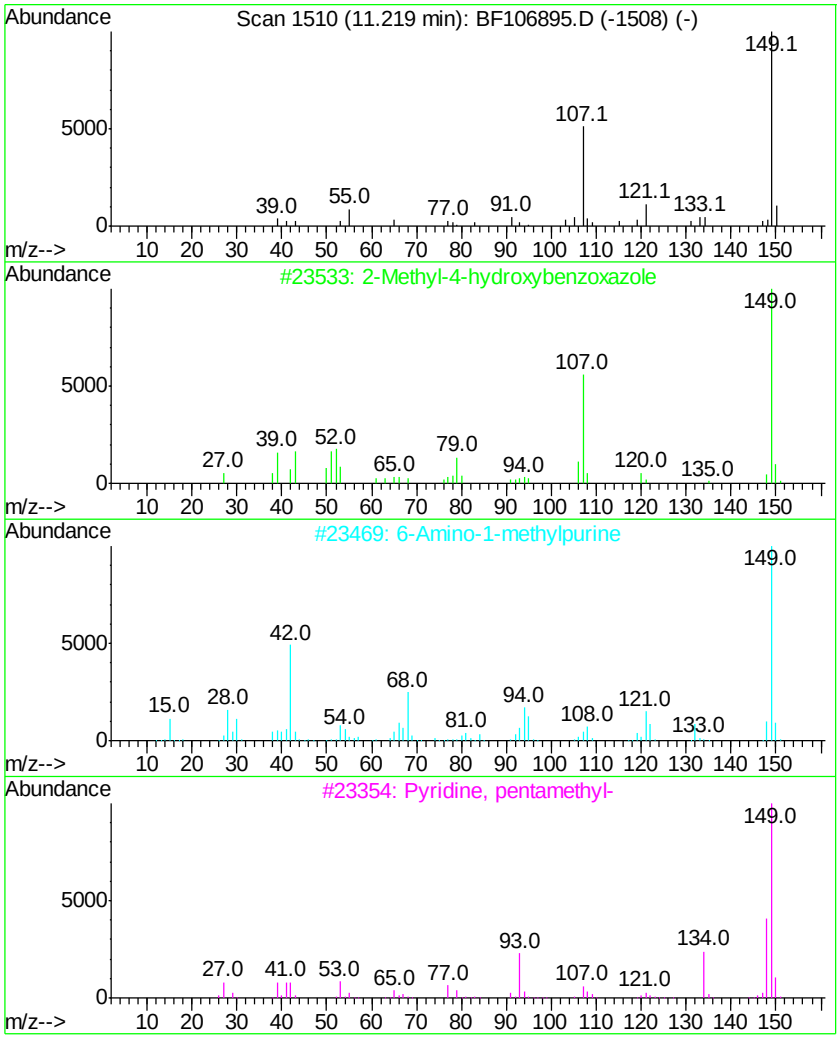
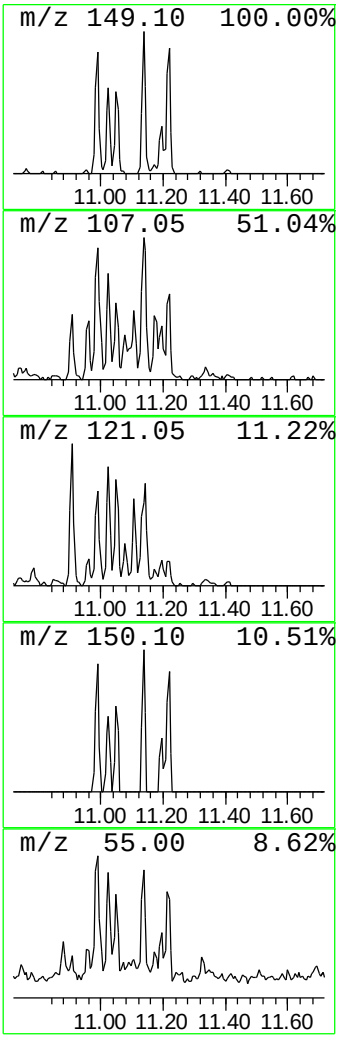
Peak Number 12 2-Methyl-4-hydroxybenzoxazole Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.22	3.38 ng	39650	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	72
2	6-Amino-1-methylpurine	149	C6H7N5	005142-22-3	40
3	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	28
4	Phthalic acid, decyl 2,7-dimethy...	440	C28H40O4	1000315-49-5	28
5	2H-1,4-Benzoxazin-3(4H)-one	149	C8H7NO2	005466-88-6	28





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Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
Sample : J3693-06
Misc :
ALS Vial : 32 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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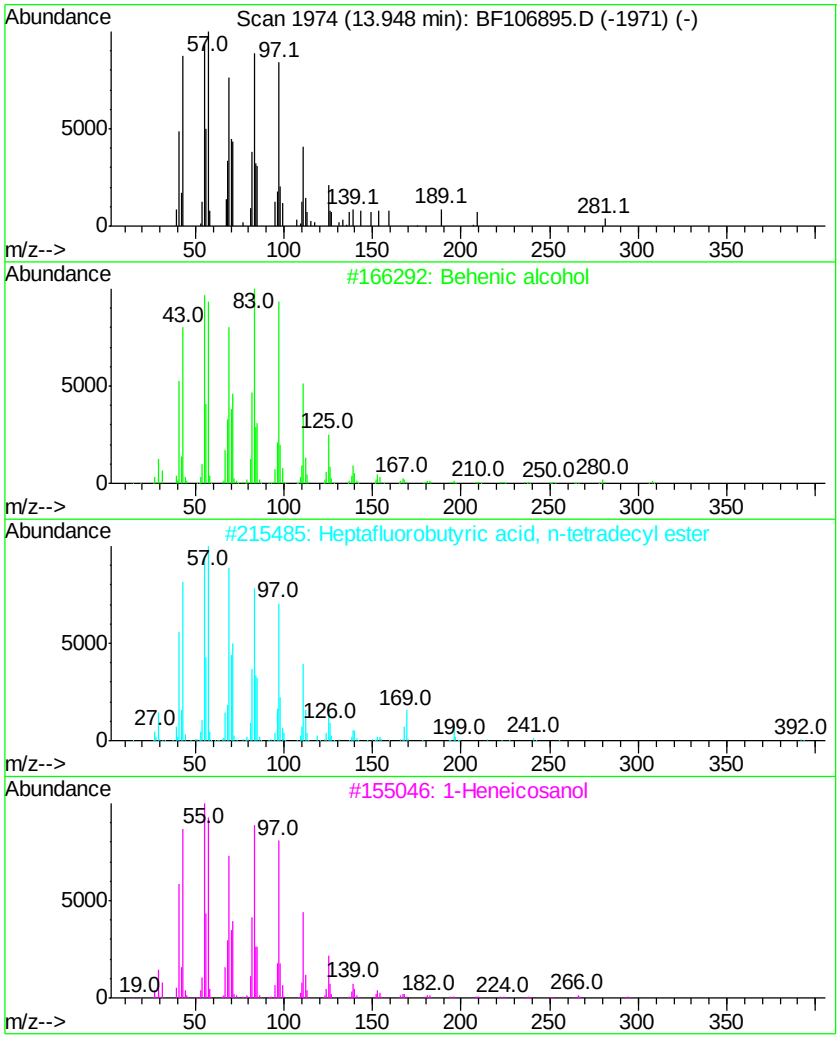
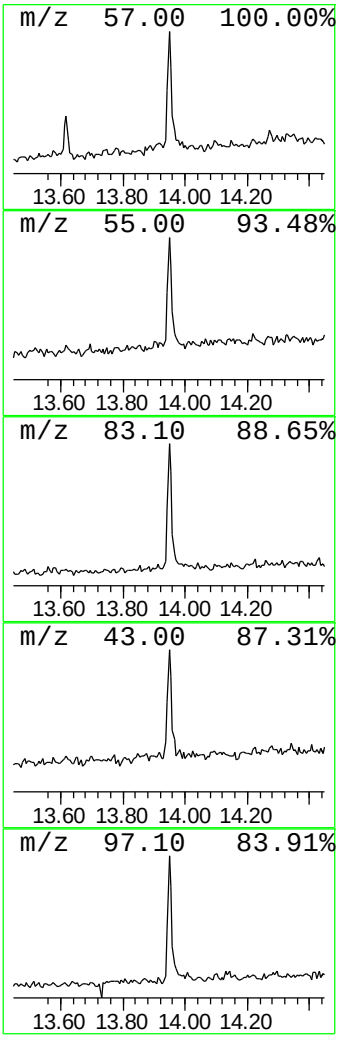
Peak Number 13 Behenic alcohol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.23 ng	51351	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	95





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062718\
Data File : BF106895.D
Acq On : 28 Jun 2018 2:28
Operator : JU/SJ
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Misc :
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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	2.3	ng	26897	1	6.95	235505	20.0
unknown6.73	6.73	70.1	ng	825539	1	6.95	235505	20.0
Acetamide, N-(2,6...	10.91	2.9	ng	34013	4	11.49	234438	20.0
4-(1,1-Dimethylpr...	10.96	6.0	ng	70101	4	11.49	234438	20.0
Benzene, [1-(1-me...	10.99	9.2	ng	107338	4	11.49	234438	20.0
Phenol, p-tert-bu...	11.02	8.1	ng	94705	4	11.49	234438	20.0
Phenol, 2-(1,1-di...	11.05	3.9	ng	45586	4	11.49	234438	20.0
Adenine	11.10	2.9	ng	33865	4	11.49	234438	20.0
5H-Pyrrolo(3,2-d)...	11.14	7.9	ng	93067	4	11.49	234438	20.0
Carbamic acid, N-...	11.17	6.6	ng	77333	4	11.49	234438	20.0
2-Methyl-4-hydrox...	11.22	3.4	ng	39650	4	11.49	234438	20.0
Behenic alcohol	13.95	3.2	ng	51351	5	14.14	318286	20.0