LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099949.D
Acq On : 29 Oct 2017 7:55
Operator : SJ/JU
Sample : I6100-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-S

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:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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	5.004	493	496	515	rBV	98320	151637	4.97%	0.852%
2	5.410	562	565	590	rBV	746477	931699	30.56%	5.233%
3	6.428	735	738	755	rBV	502225	638256	20.94%	3.585%
4	6.557	757	760	767	rVB	1741358	1602538	52.57%	9.001%
5	6.787	796	799	809	rBV	679934	608042	19.95%	3.415%
6	6.939	821	825	847	rBV	2199398	2200744	72.20%	12.360%
7	7.357	892	896	913	rBV	1497669	1672007	54.85%	9.391%
8	8.069	1013	1017	1035	rBV	918683	808610	26.53%	4.542%
9	8.628	1109	1112	1121	rBV	87262	78614	2.58%	0.442%
10	9.145	1195	1200	1203	rBV	3141330	3048323	100.00%	17.121%
11	9.539	1264	1267	1277	rBB	83650	69593	2.28%	0.391%
12	9.822	1309	1315	1327	rVB	961376	811648	26.63%	4.559%
13	10.492	1425	1429	1433	rBV	91328	70018	2.30%	0.393%
14	10.533	1433	1436	1446	rVB	344984	272403	8.94%	1.530%
15	10.616	1447	1450	1462	rBV	888911	805138	26.41%	4.522%
16	11.316	1565	1569	1577	rBV	625829	610687	20.03%	3.430%
17	12.698	1801	1804	1808	rBV	178967	150398	4.93%	0.845%
18	12.898	1833	1838	1841	rBV	2140761	1938295	63.59%	10.886%
19	13.404	1921	1924	1928	rBV	122675	96490	3.17%	0.542%
20	13.774	1984	1987	1994	rBV	45302	52245	1.71%	0.293%
21	13.963	2015	2019	2028	rBV	566304	519623	17.05%	2.918%
22	15.421	2263	2267	2278	rVB	370566	502155	16.47%	2.820%
23	15.804	2327	2332	2337	rVB2	26840	38600	1.27%	0.217%
24	16.286	2409	2414	2419	rBV2	26471	43615	1.43%	0.245%
25	16.851	2504	2510	2519	rVB4	20607	43572	1.43%	0.245%
26	17.515	2617	2623	2632	rVB5	17347	39706	1.30%	0.223%

Sum of corrected areas: 17804656

LSC Report - Integrated Chromatogram

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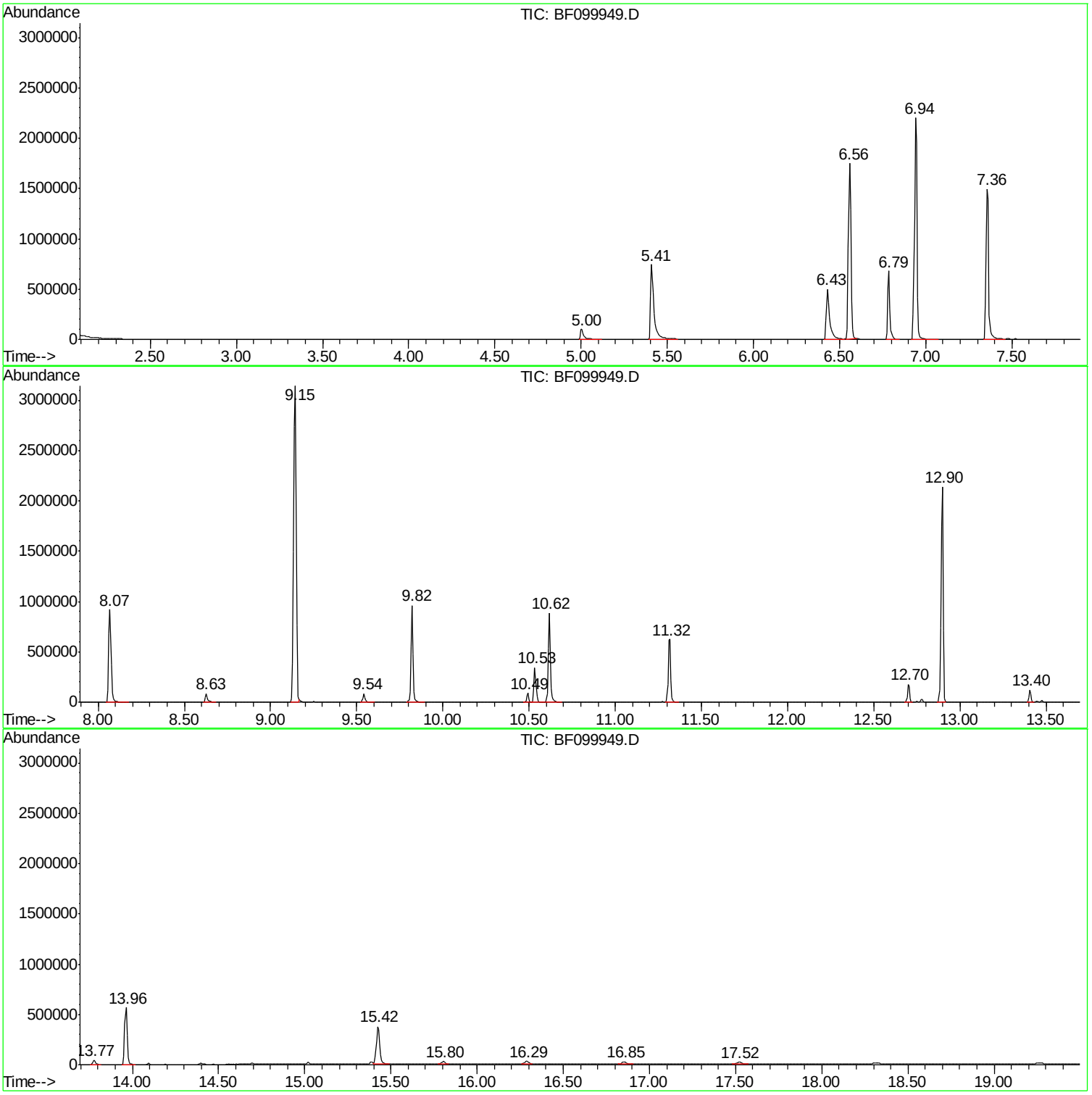
Operator : SJ/JU
Sample : I6100-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099949.D
Acq On : 29 Oct 2017 7:55
Operator : SJ/JU
Sample : I6100-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
102317-TIDO-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

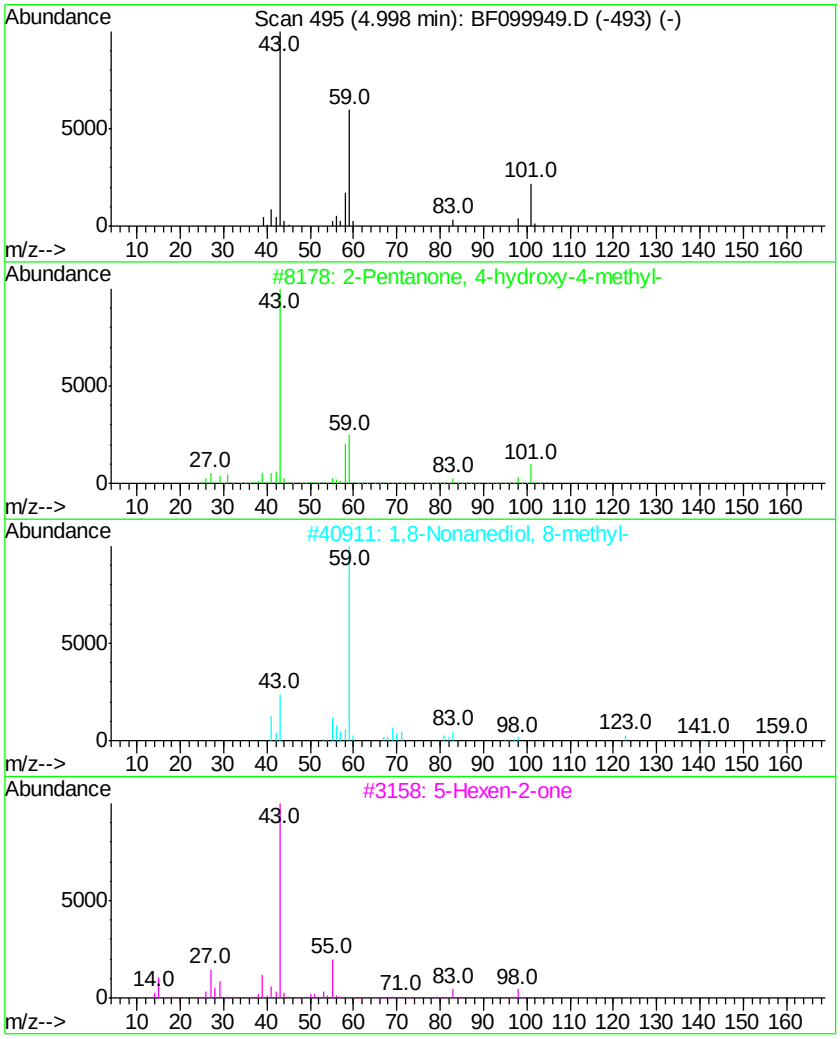
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

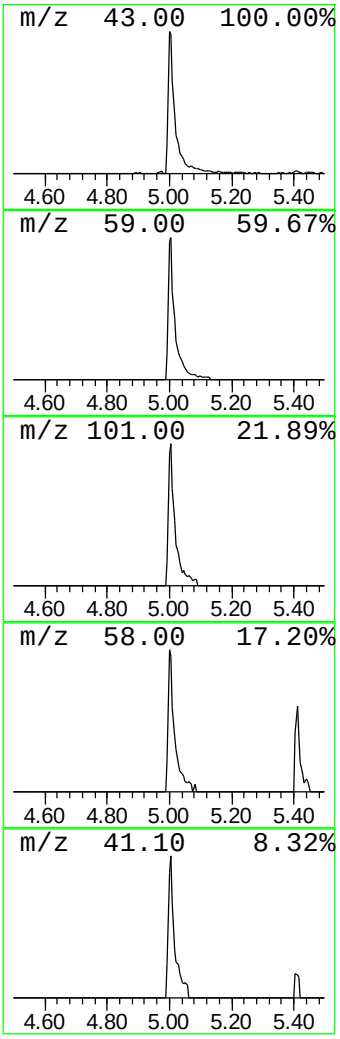
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	4.99 ng	151637	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Data File : BF099949.D
Acq On : 29 Oct 2017 7:55
Operator : SJ/JU
Sample : I6100-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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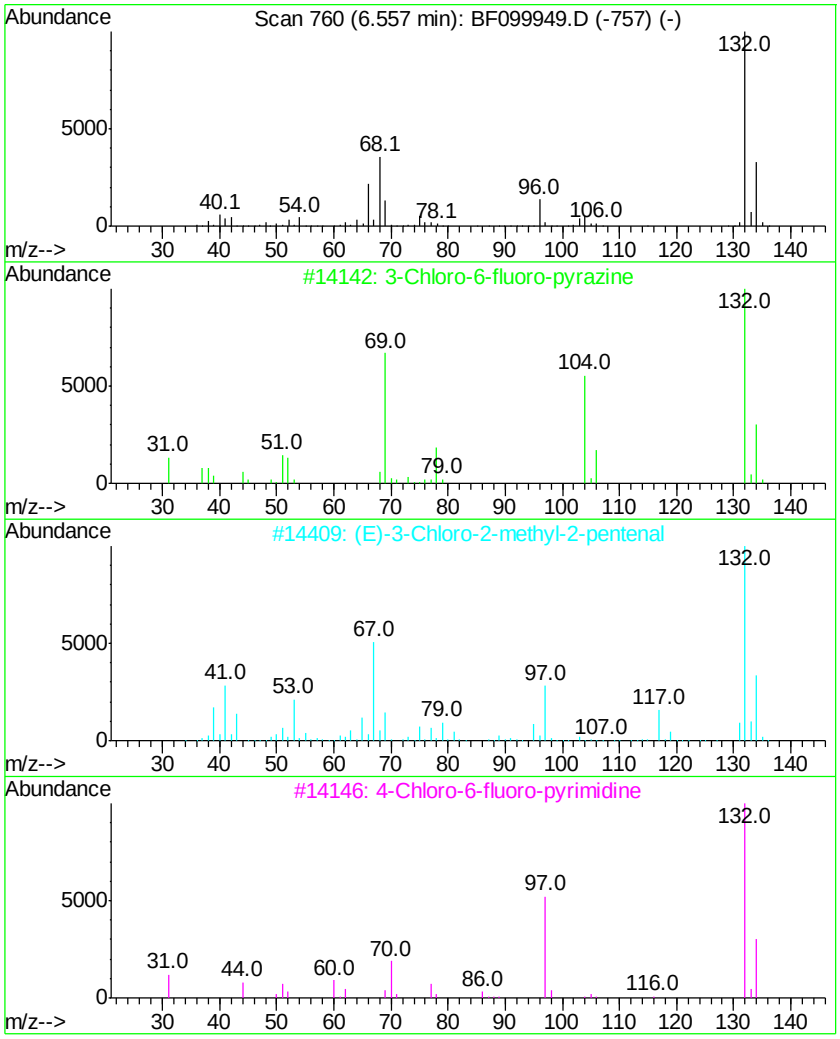
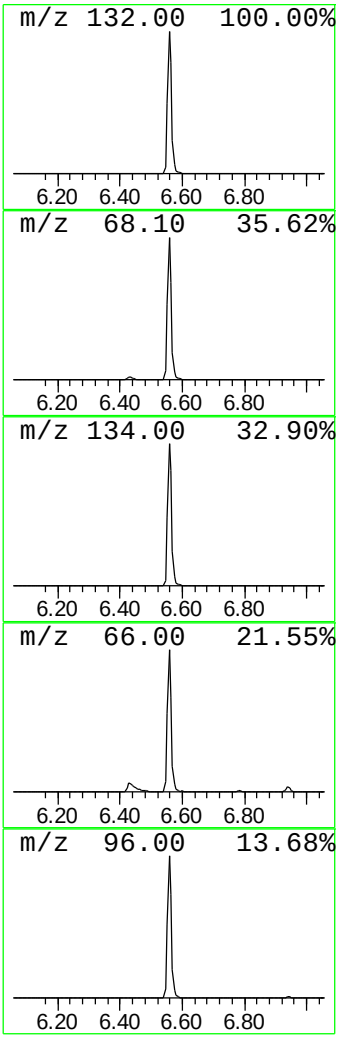
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	52.71 ng	1602540	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	5-Aminoindole	132	C8H8N2	005192-03-0	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099949.D
Acq On : 29 Oct 2017 7:55
Operator : SJ/JU
Sample : I6100-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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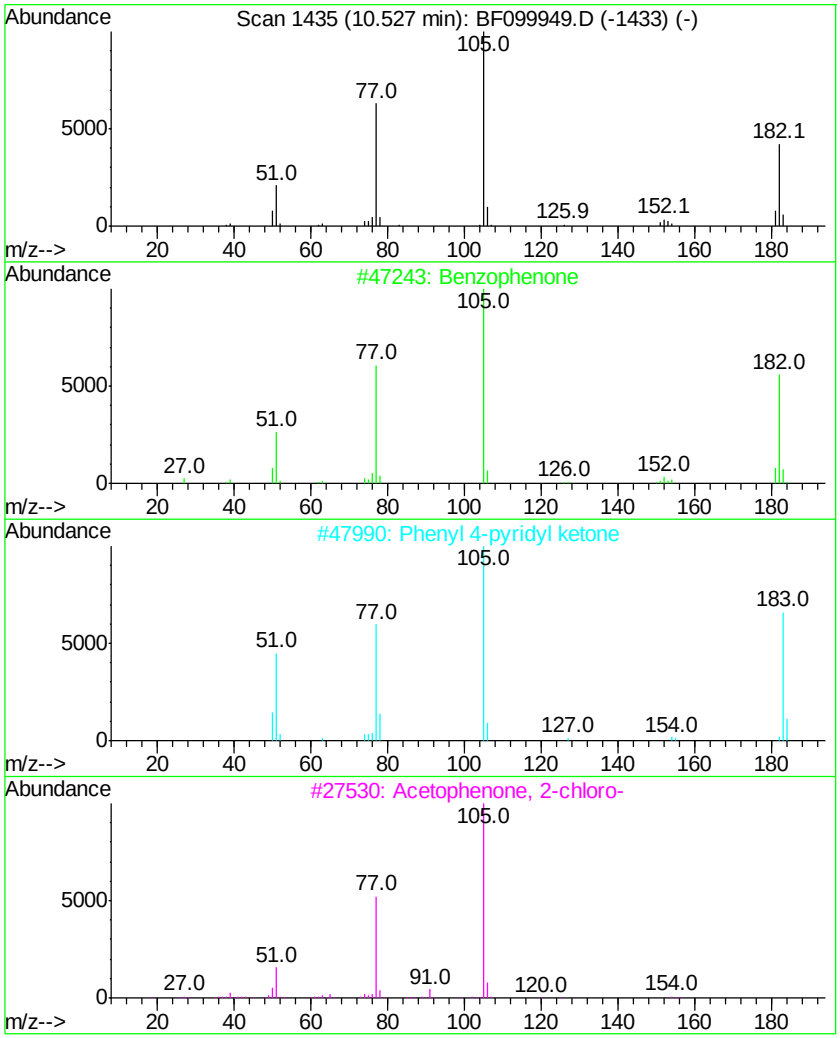
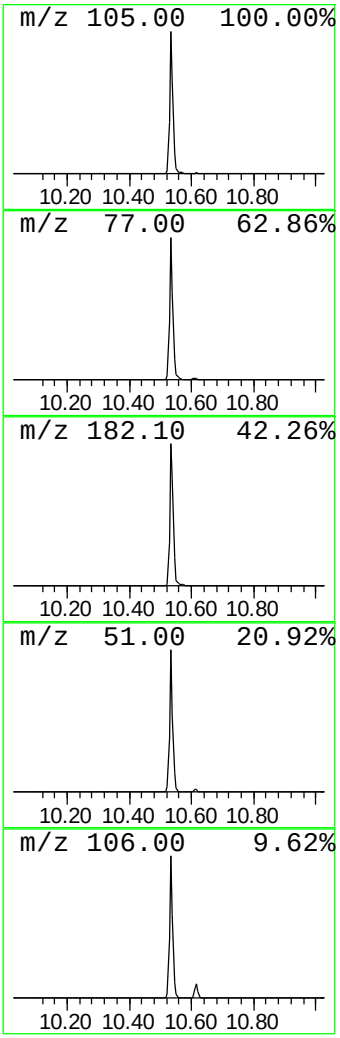
Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	6.71 ng	272403	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
4	Benzopinacol	366	C26H22O2	000464-72-2	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099949.D
Acq On : 29 Oct 2017 7:55
Operator : SJ/JU
Sample : I6100-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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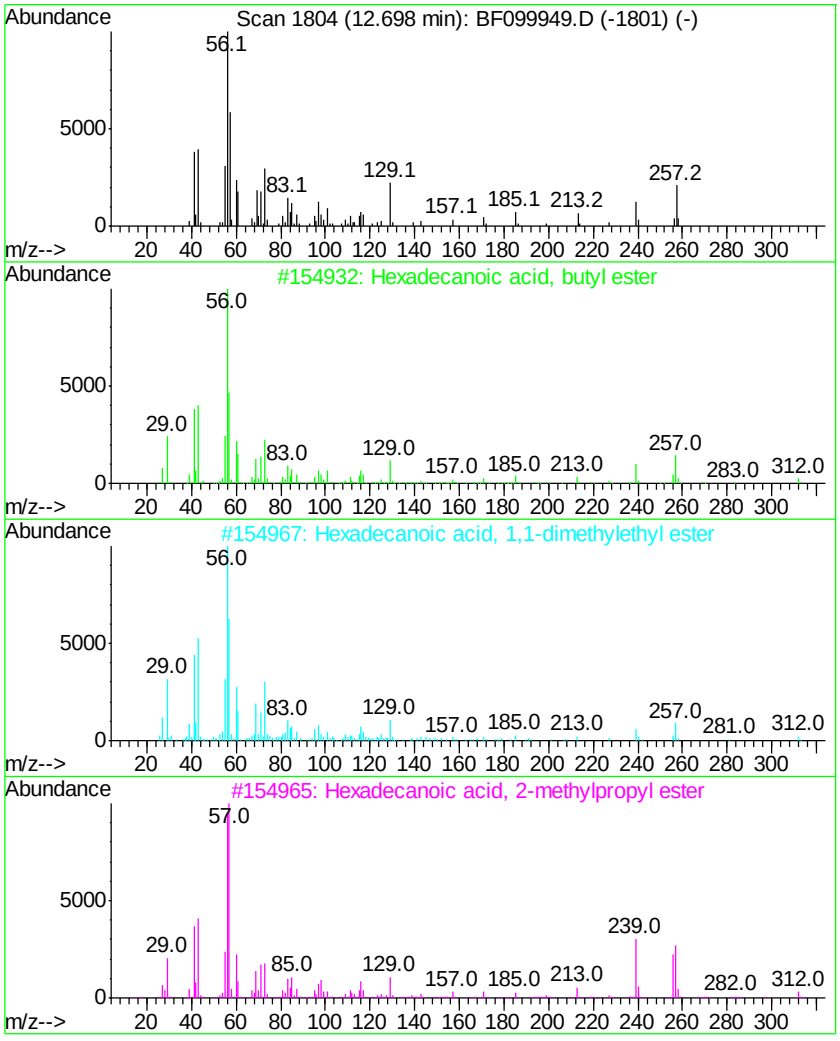
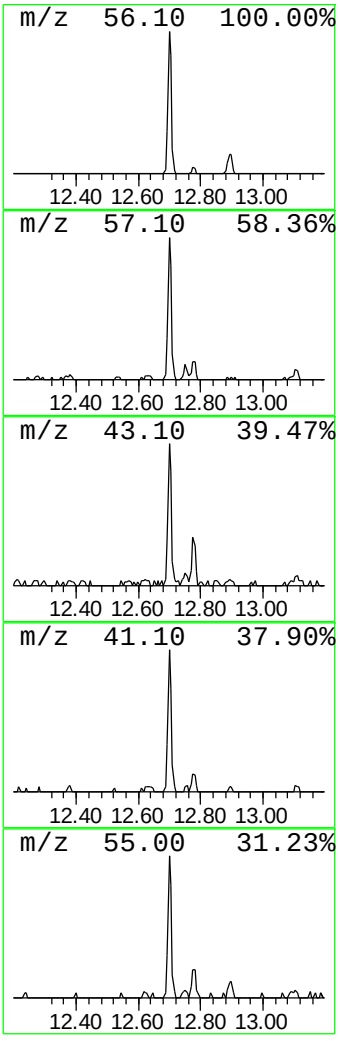
Peak Number 5 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	5.79 ng	150398	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	74
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	50
4	Nipecotic acid	129	C6H11NO2	000498-95-3	37
5	Trifluoroacetic acid, 4-methylpe...	198	C8H13F3O2	000327-71-9	35





Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099949.D
Acq On : 29 Oct 2017 7:55
Operator : SJ/JU
Sample : I6100-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

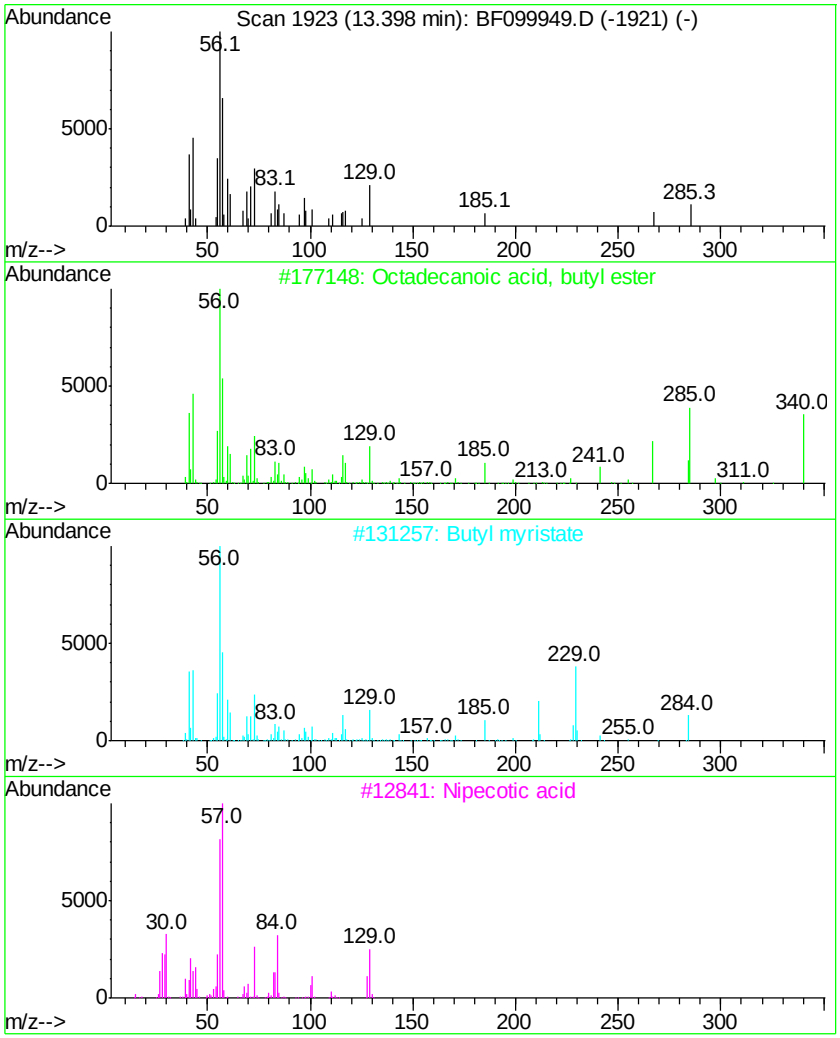
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

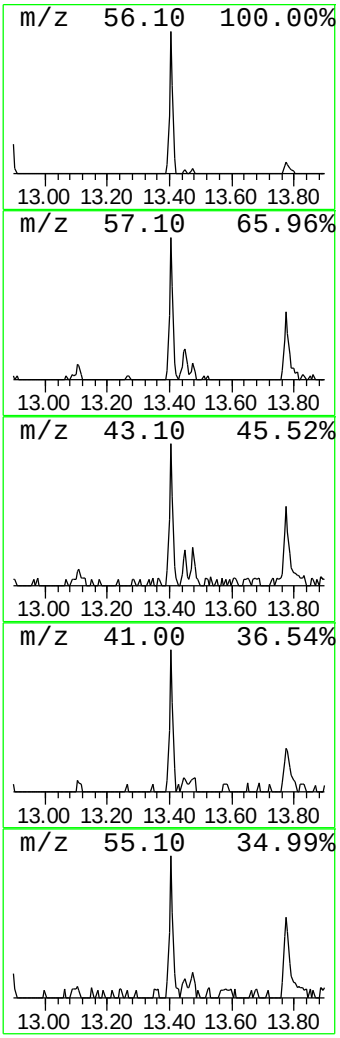
****

Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	3.71 ng	96490	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2	Butyl myristate	284	C18H36O2	000110-36-1	80
3	Nipecotic acid	129	C6H11NO2	000498-95-3	50
4	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	38
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35





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Operator : SJ/JU
Sample : I6100-04
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-U-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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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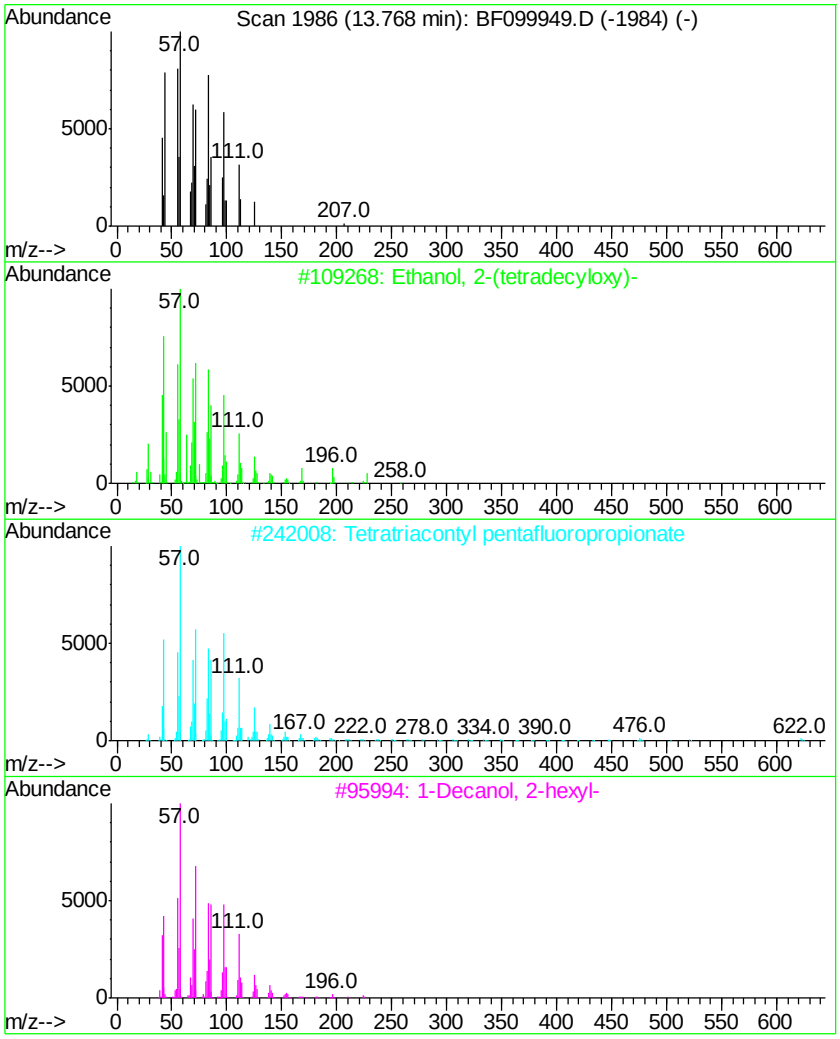
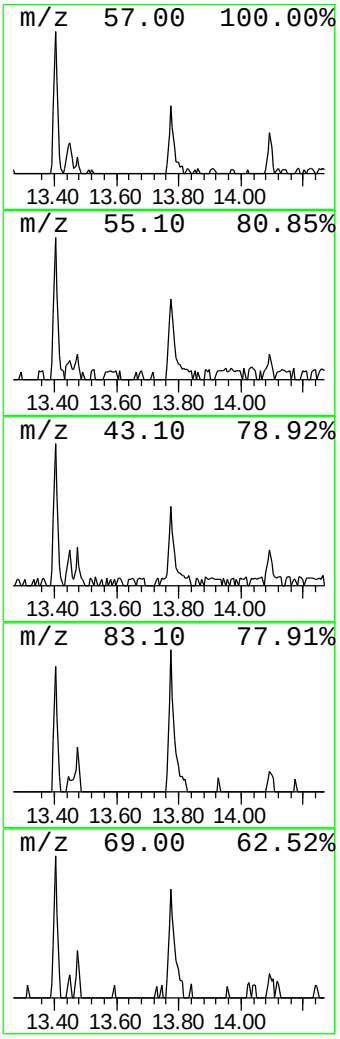
Peak Number 7 Ethanol, 2-(tetradecyloxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.01 ng	52245	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	87
3	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87
4	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	87
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	83





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.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...	5.00	5.0	ng	151637	1	6.79	608042	20.0
unknown6.56	6.56	52.7	ng	1602540	1	6.79	608042	20.0
Benzophenone	10.53	6.7	ng	272403	3	9.82	811648	20.0
Hexadecanoic acid...	12.70	5.8	ng	150398	5	13.96	519623	20.0
Octadecanoic acid...	13.40	3.7	ng	96490	5	13.96	519623	20.0
Ethanol, 2-(tetra...	13.77	2.0	ng	52245	5	13.96	519623	20.0