LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101617\
Data File : BF099541.D
Acq On : 16 Oct 2017 13:45
Operator : SJ/JU
Sample : I5776-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-104-2(5-10)

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-BF092317.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	5.075	505	508	522	rBV	313354	492569	16.07%	2.010%
2	5.475	571	576	579	rBV	2643797	2694119	87.91%	10.995%
3	6.487	742	748	760	rBV	2414648	2873882	93.78%	11.729%
4	6.616	766	770	774	rBV	2715095	2835468	92.53%	11.572%
5	6.845	805	809	817	rVB	649003	588931	19.22%	2.403%
6	6.998	831	835	839	rBV	2376560	2245463	73.27%	9.164%
7	7.410	900	905	908	rBV	1707940	1763531	57.55%	7.197%
8	8.122	1022	1026	1036	rBV	855359	802538	26.19%	3.275%
9	8.681	1117	1121	1131	rBV	140283	117776	3.84%	0.481%
10	9.198	1204	1209	1213	rBV	3001414	3064523	100.00%	12.507%
11	9.592	1272	1276	1284	rBV	465347	361365	11.79%	1.475%
12	9.880	1321	1325	1329	rBV	1006674	837950	27.34%	3.420%
13	10.592	1443	1446	1450	rBV	439967	355034	11.59%	1.449%
14	10.675	1455	1460	1463	rBV	1611098	1504551	49.10%	6.140%
15	11.369	1574	1578	1581	rBV	891963	724926	23.66%	2.959%
16	12.951	1843	1847	1850	rBV	2217142	2077727	67.80%	8.479%
17	13.833	1992	1997	2005	rBV	72702	103898	3.39%	0.424%
18	14.010	2023	2027	2031	rBV	555191	506881	16.54%	2.069%
19	15.486	2272	2278	2285	rBV	427136	551988	18.01%	2.253%

Sum of corrected areas: 24503120

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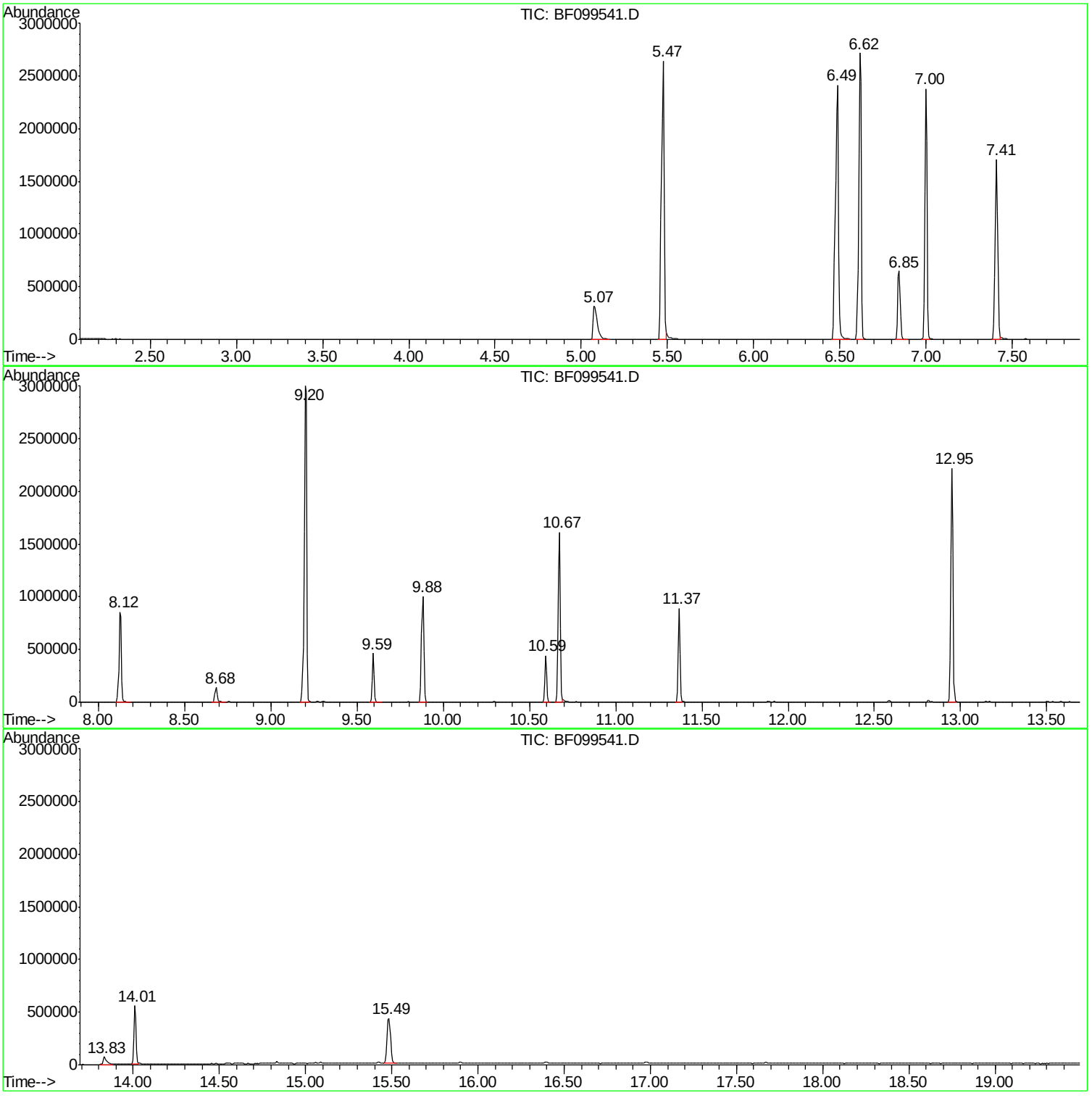
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
ENV-104-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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

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Data File : BF099541.D
Acq On : 16 Oct 2017 13:45
Operator : SJ/JU
Sample : I5776-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : ENV-104-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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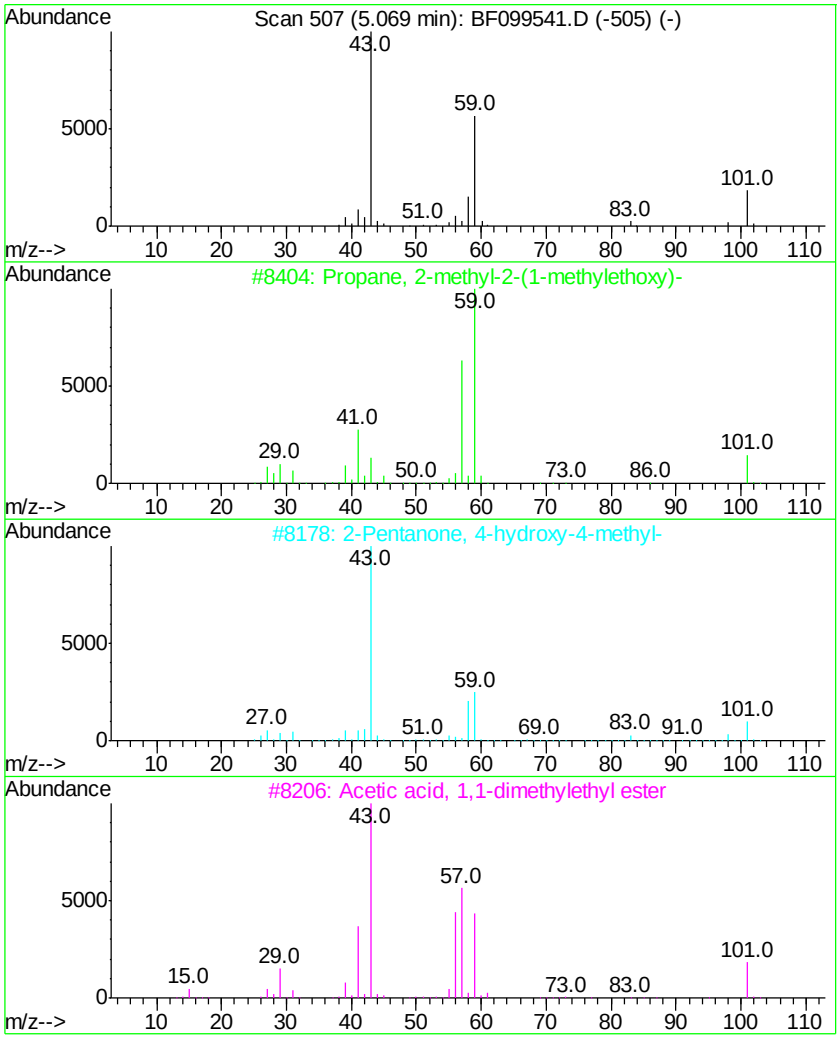
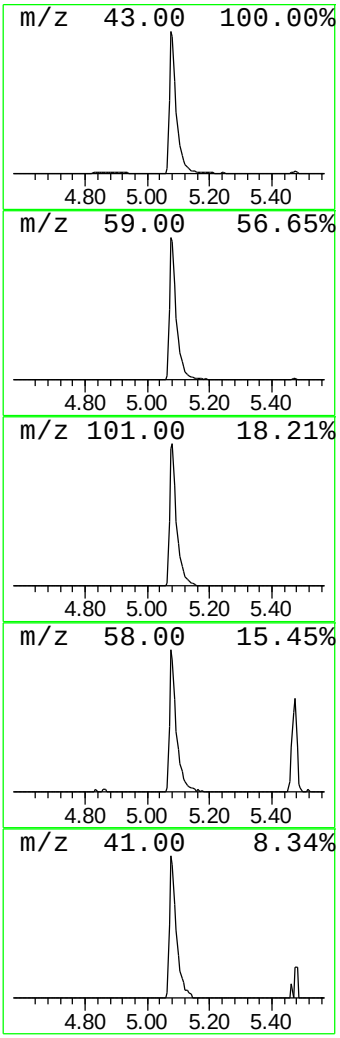
Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	16.73 ng	492569	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Instrument : BNA_F
ClientSampleId : ENV-104-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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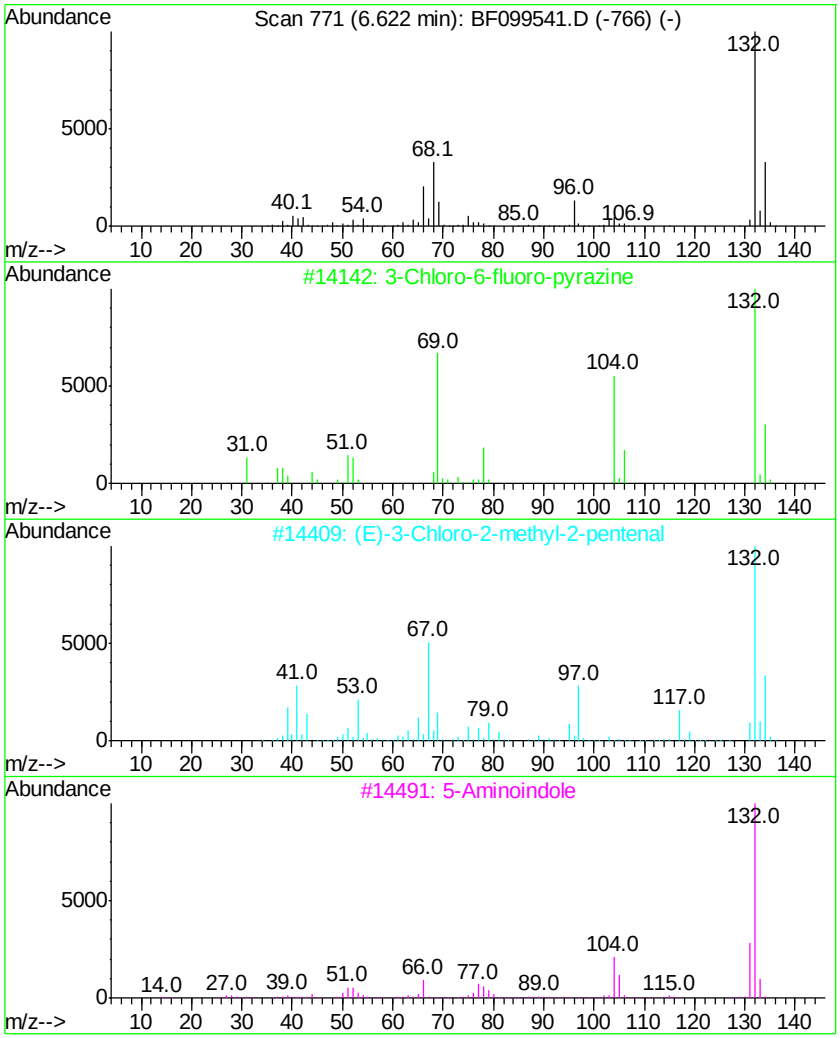
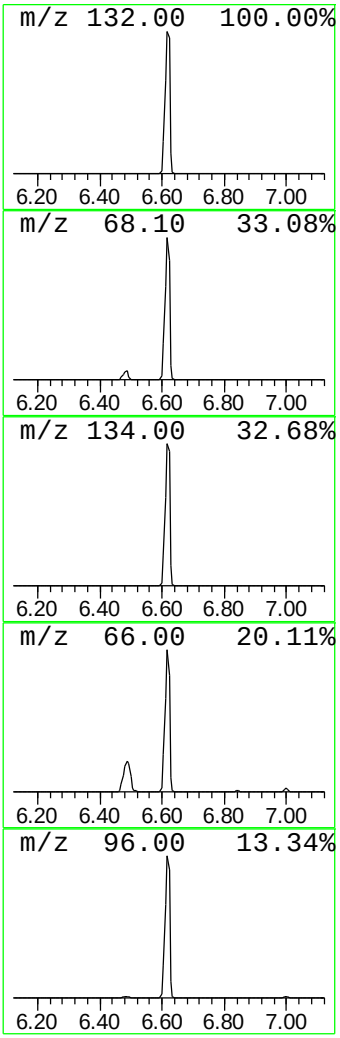
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	96.29 ng	2835470	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Misc :
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Instrument : BNA_F
ClientSampleId : ENV-104-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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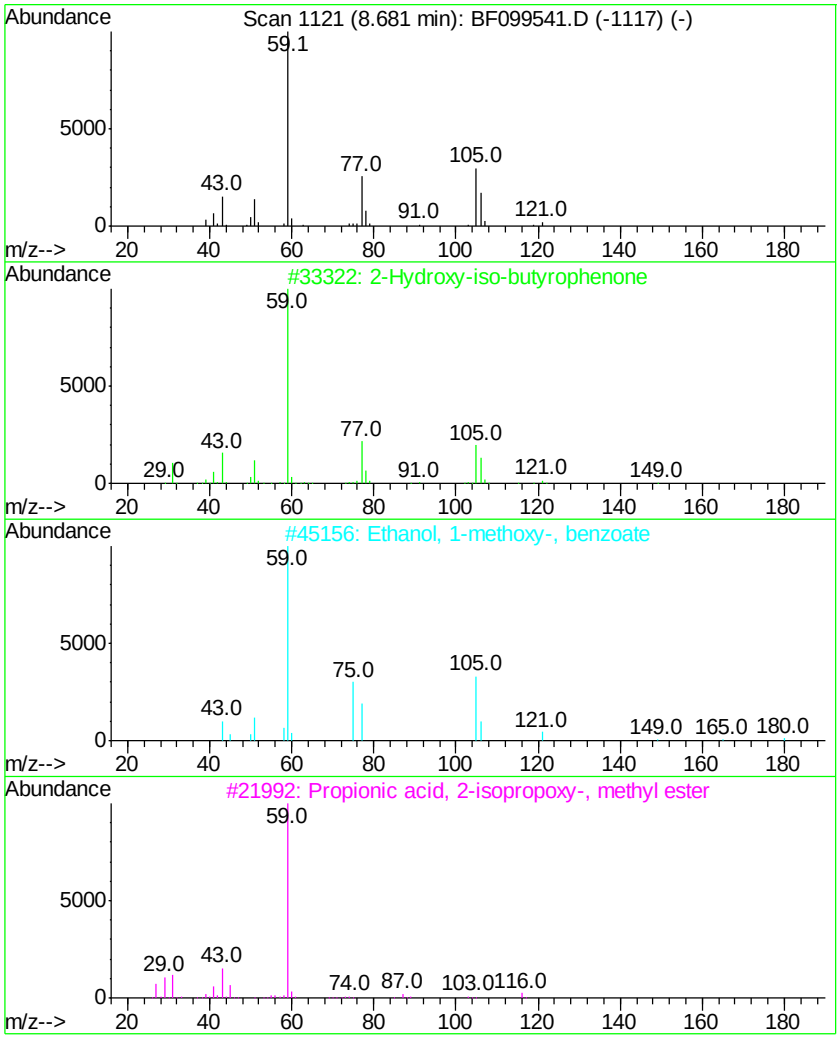
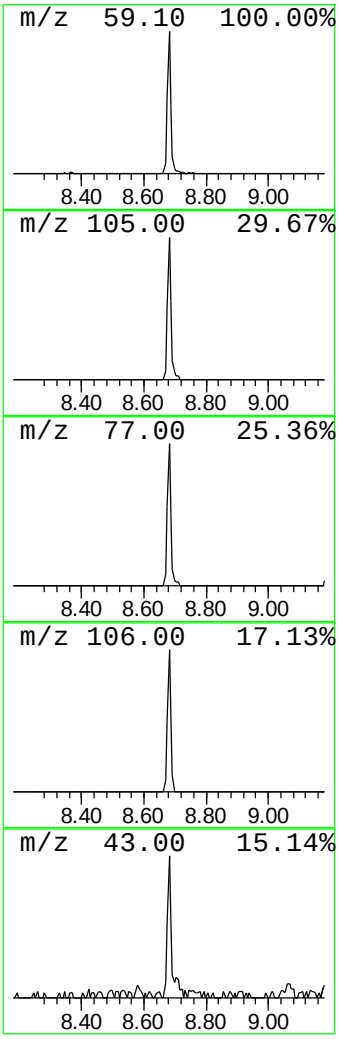
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.68	2.94 ng	117776	Naphthalene-d8	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	72
3	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4	Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	9
5	Guanidine	59	CH5N3	000113-00-8	7





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Misc :
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Instrument : BNA_F
ClientSampleId : ENV-104-2(5-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.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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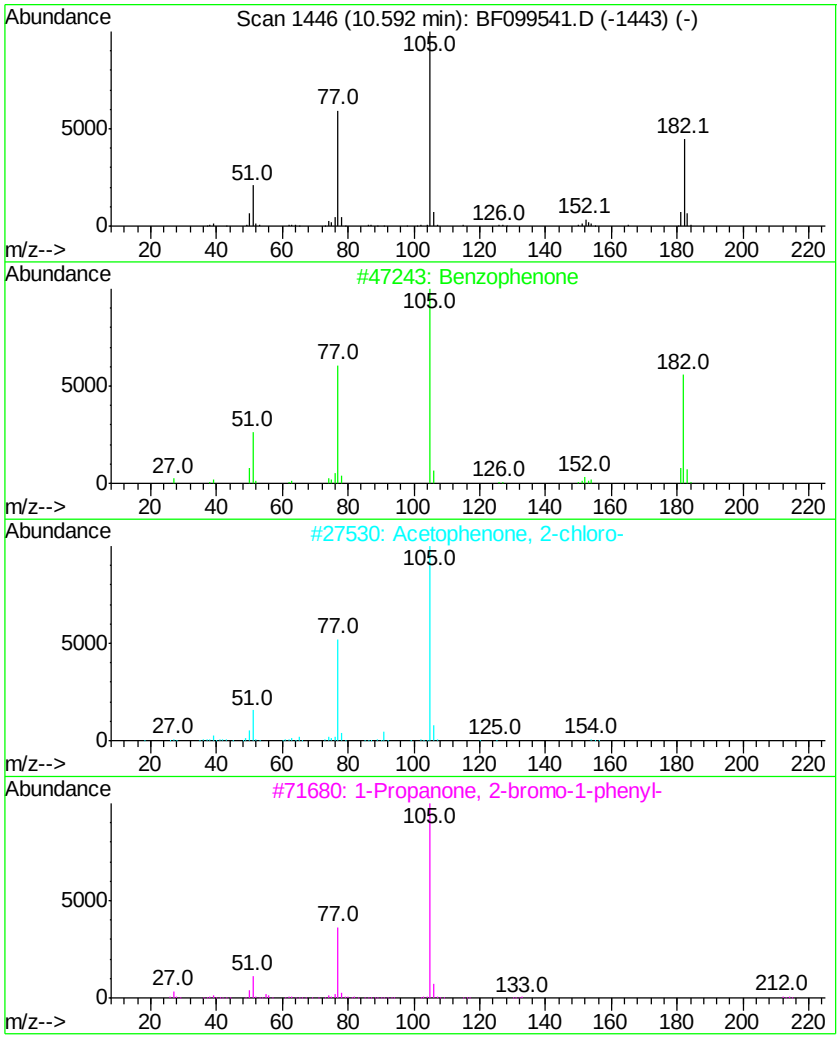
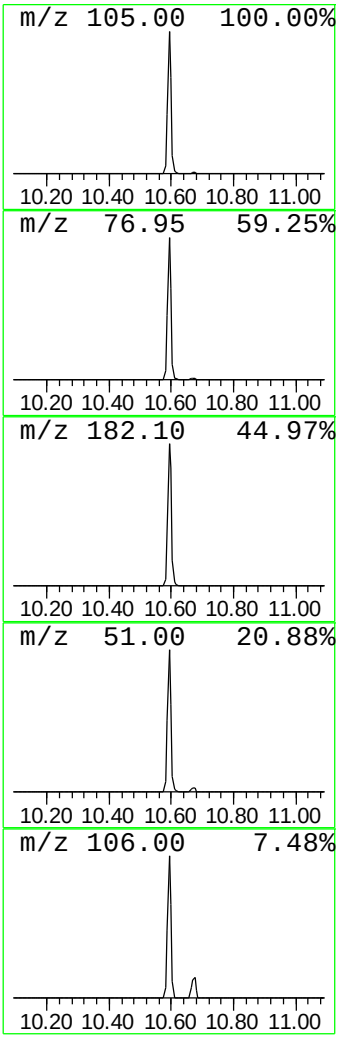
Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	8.47 ng	355034	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	47
5	Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	47





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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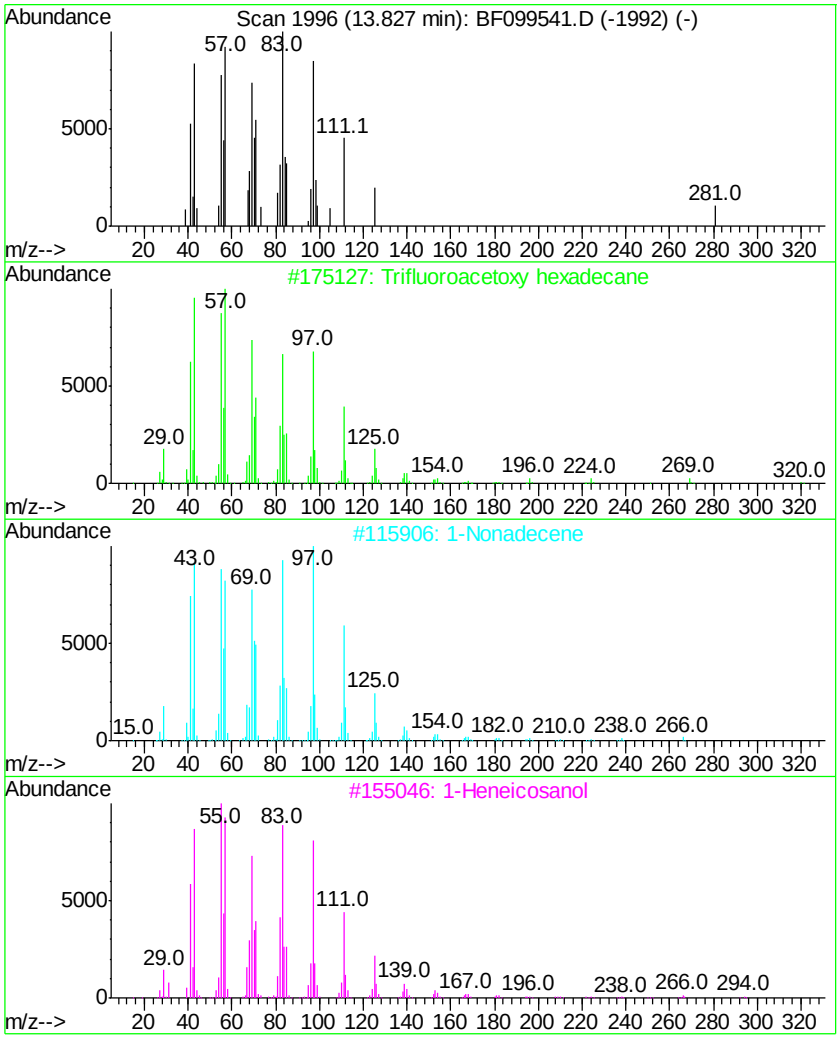
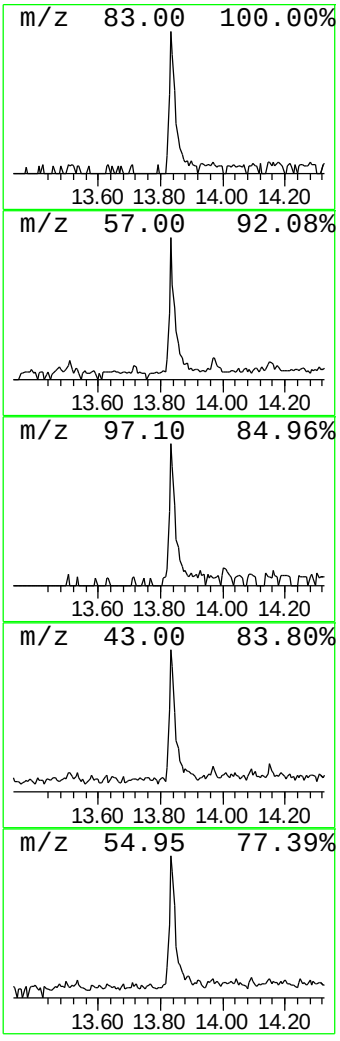
****

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.10 ng	103898	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	1-Nonadecene	266	C19H38	018435-45-5	91
3	1-Heneicosanol	312	C21H44O	015594-90-8	91
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91





Tentatively Identified Compound (LSC) summary

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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
Propane, 2-methyl...	5.07	16.7	ng	492569	1	6.85	588931	20.0
unknown6.62	6.62	96.3	ng	2835470	1	6.85	588931	20.0
2-Hydroxy-iso-but...	8.68	2.9	ng	117776	2	8.12	802538	20.0
Benzophenone	10.59	8.5	ng	355034	3	9.88	837950	20.0
Trifluoroacetoxy ...	13.83	4.1	ng	103898	5	14.01	506881	20.0