LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099527.D
Acq On : 15 Oct 2017 21:36
Operator : SJ/JU
Sample : I5821-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPSB-6B-18-18.5-BGS

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	5.069	503	507	518	rBV	243323	315183	17.30%	2.049%
2	5.469	571	575	591	rBV	1886319	1789537	98.22%	11.635%
3	6.481	743	747	759	rBV	1827411	1806001	99.12%	11.742%
4	6.616	766	770	773	rBV	2107553	1822059	100.00%	11.847%
5	6.845	805	809	817	rBB	525770	450068	24.70%	2.926%
6	6.998	831	835	839	rBV	1678786	1411584	77.47%	9.178%
7	7.410	901	905	908	rBV	1170718	1037779	56.96%	6.748%
8	8.122	1023	1026	1041	rBV	584555	551700	30.28%	3.587%
9	8.681	1118	1121	1131	rBB	138386	110249	6.05%	0.717%
10	9.198	1205	1209	1212	rBV	2099828	1721290	94.47%	11.192%
11	9.592	1273	1276	1285	rBV	308760	231025	12.68%	1.502%
12	9.881	1321	1325	1332	rVB	581176	491290	26.96%	3.194%
13	10.592	1442	1446	1449	rBV	467220	346774	19.03%	2.255%
14	10.669	1456	1459	1469	rBV	843565	757856	41.59%	4.928%
15	11.369	1575	1578	1582	rBV	504900	395954	21.73%	2.574%
16	12.951	1843	1847	1850	rBV	1463111	1211806	66.51%	7.879%
17	13.833	1994	1997	2005	rBV2	32276	47409	2.60%	0.308%
18	14.010	2024	2027	2034	rBV	479970	450975	24.75%	2.932%
19	15.486	2272	2278	2284	rBV	326490	431542	23.68%	2.806%

Sum of corrected areas: 15380081

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Misc :
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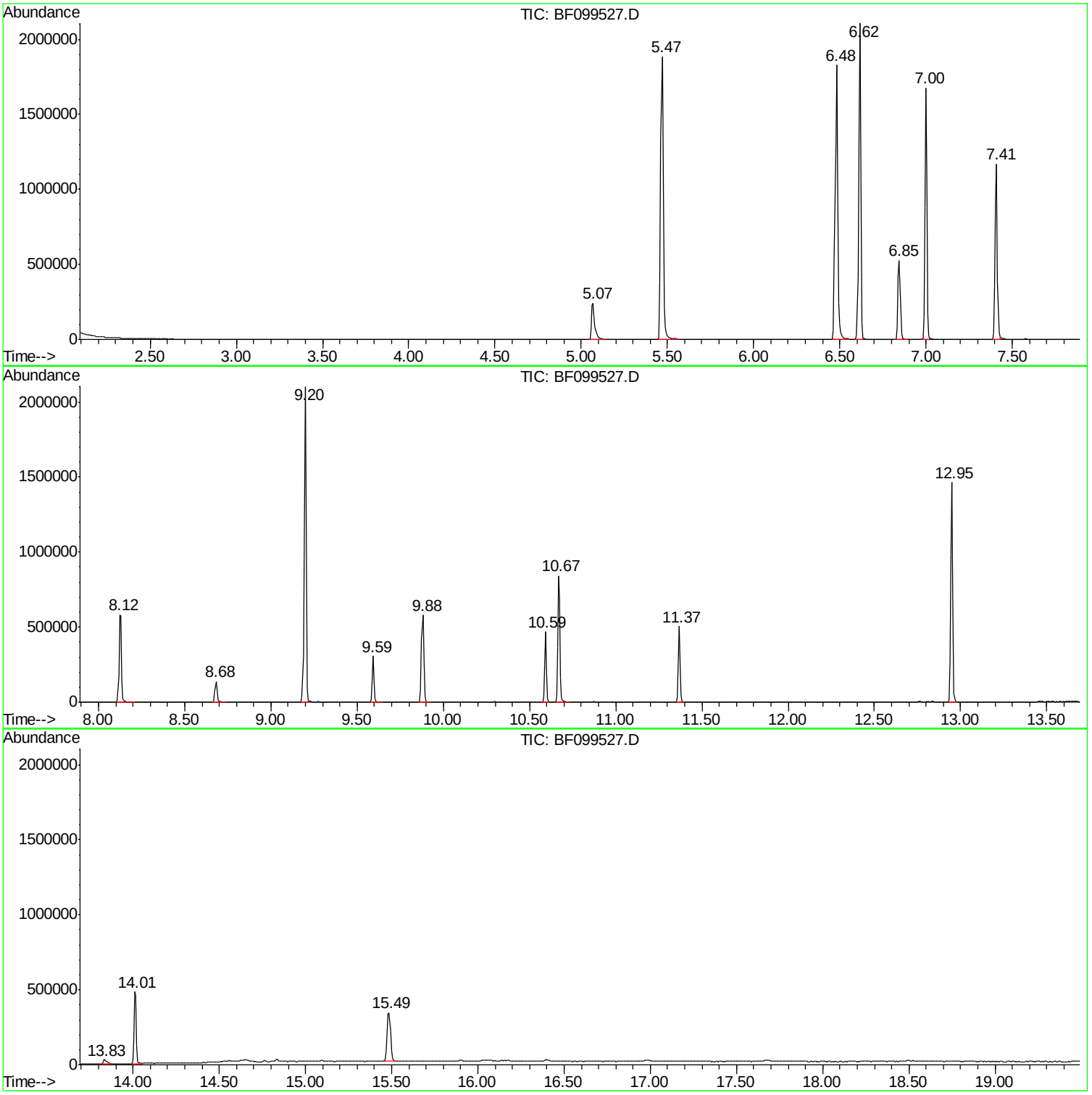
Instrument :
BNA_F
ClientSampleId :
WPSB-6B-18-18.5-BGS

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

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101517\
Data File : BF099527.D
Acq On : 15 Oct 2017 21:36
Operator : SJ/JU
Sample : I5821-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPSB-6B-18-18.5-BGS

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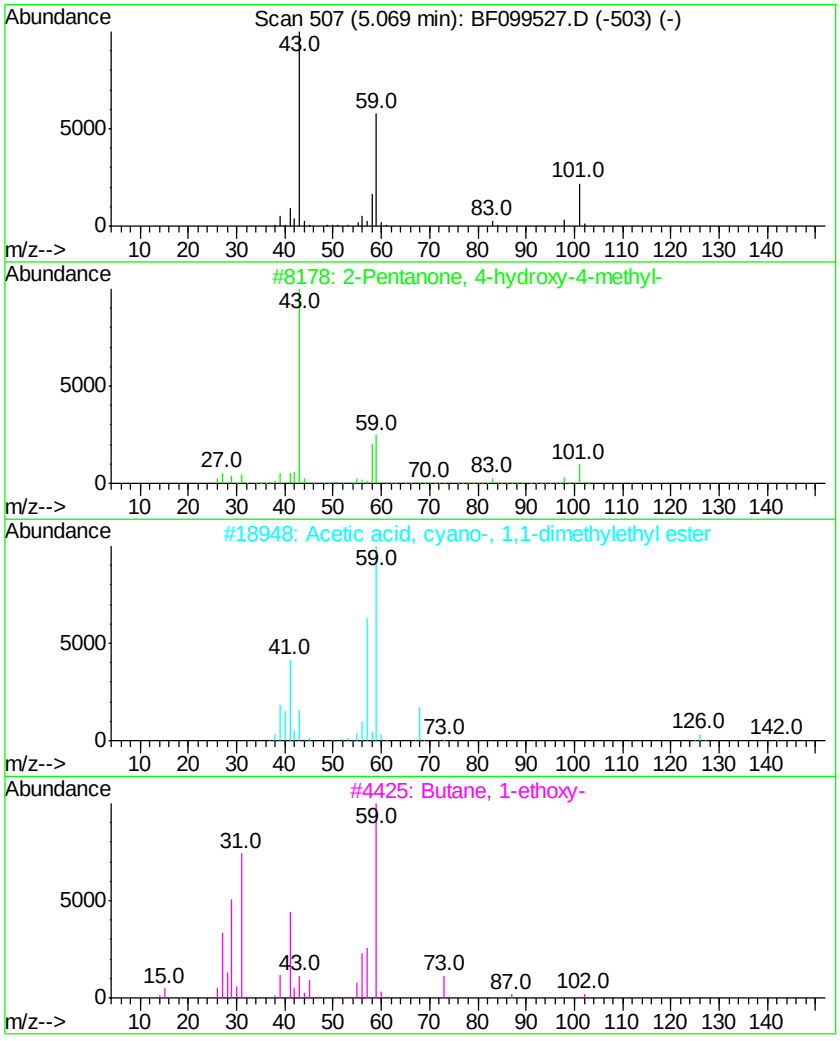
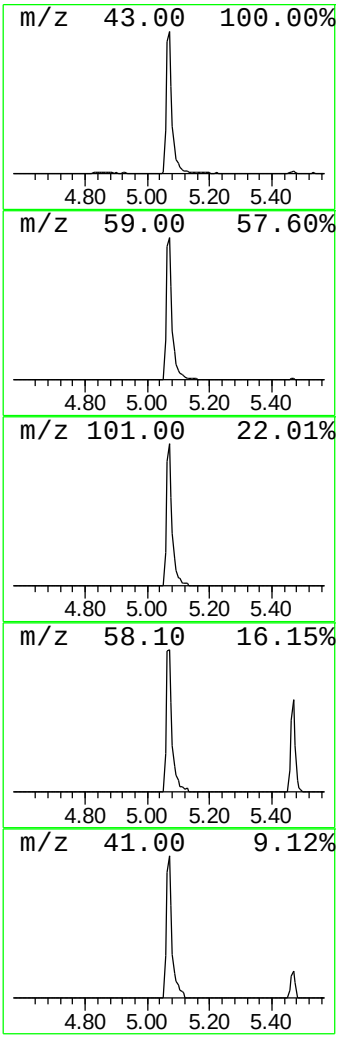
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	14.01 ng	315183	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Instrument : BNA_F
ClientSampleId : WPSB-6B-18-18.5-BGS

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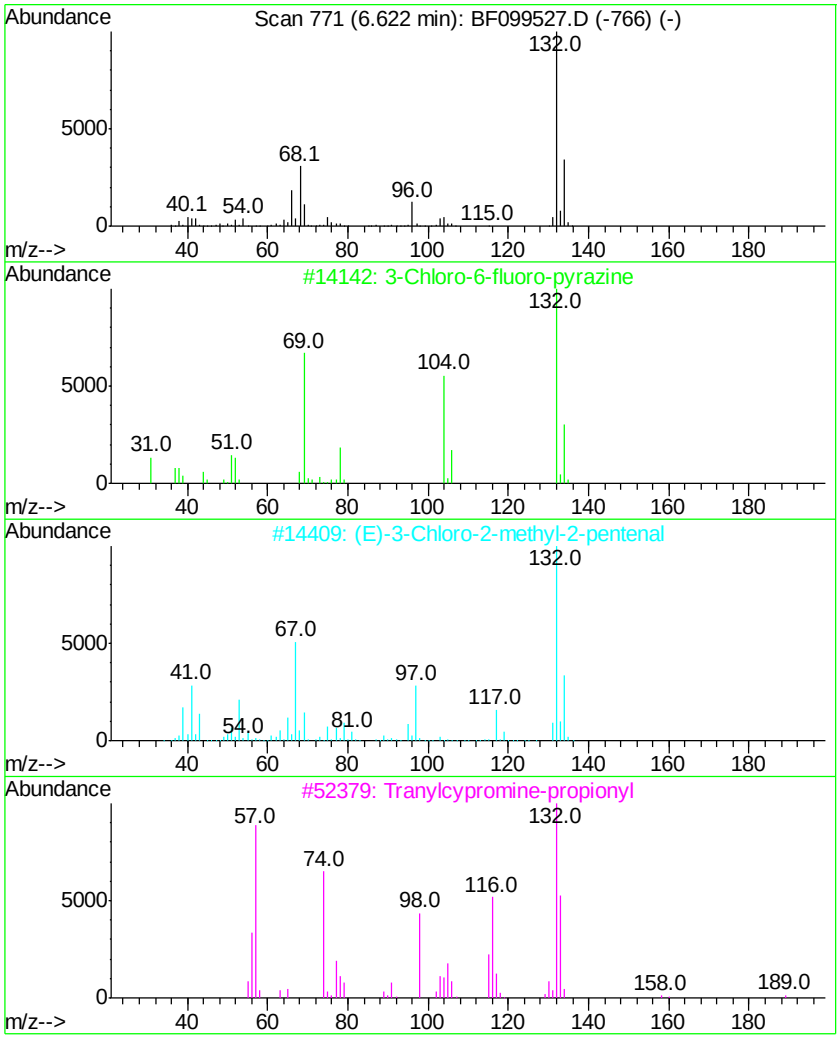
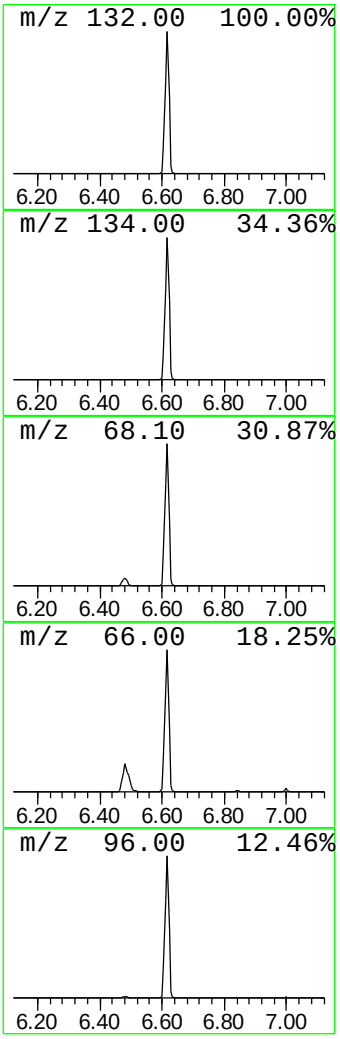
Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	80.97 ng	1822060	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	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Xenon	132	Xe	007440-63-3	9





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Misc :
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Instrument : BNA_F
ClientSampleId : WPSB-6B-18-18.5-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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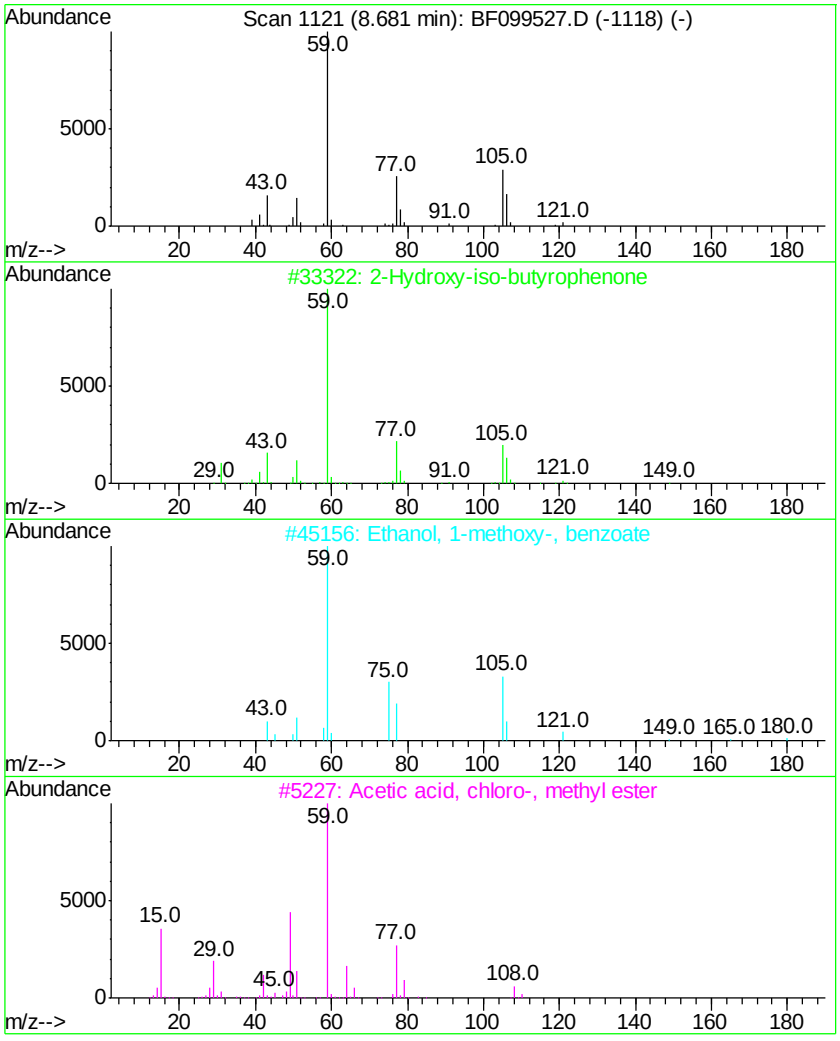
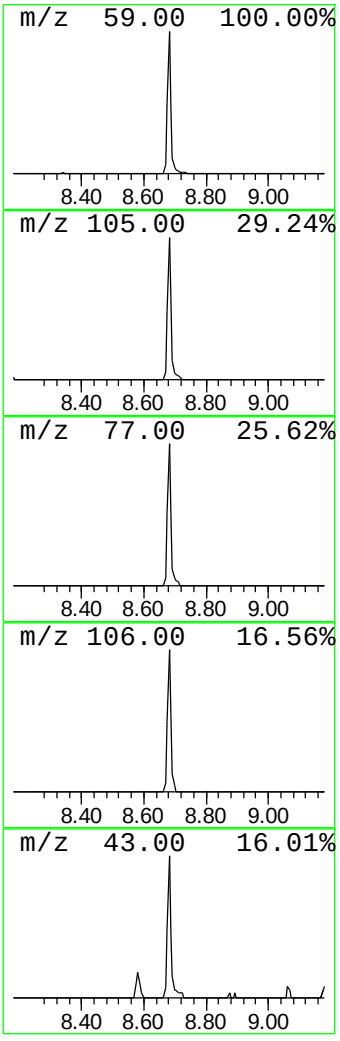
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.68	4.00 ng	110249	Naphthalene-d8	8.13

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	56
3	Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	9
4	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
5	Guanidine	59	CH5N3	000113-00-8	7





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Operator : SJ/JU
Sample : I5821-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPSB-6B-18-18.5-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
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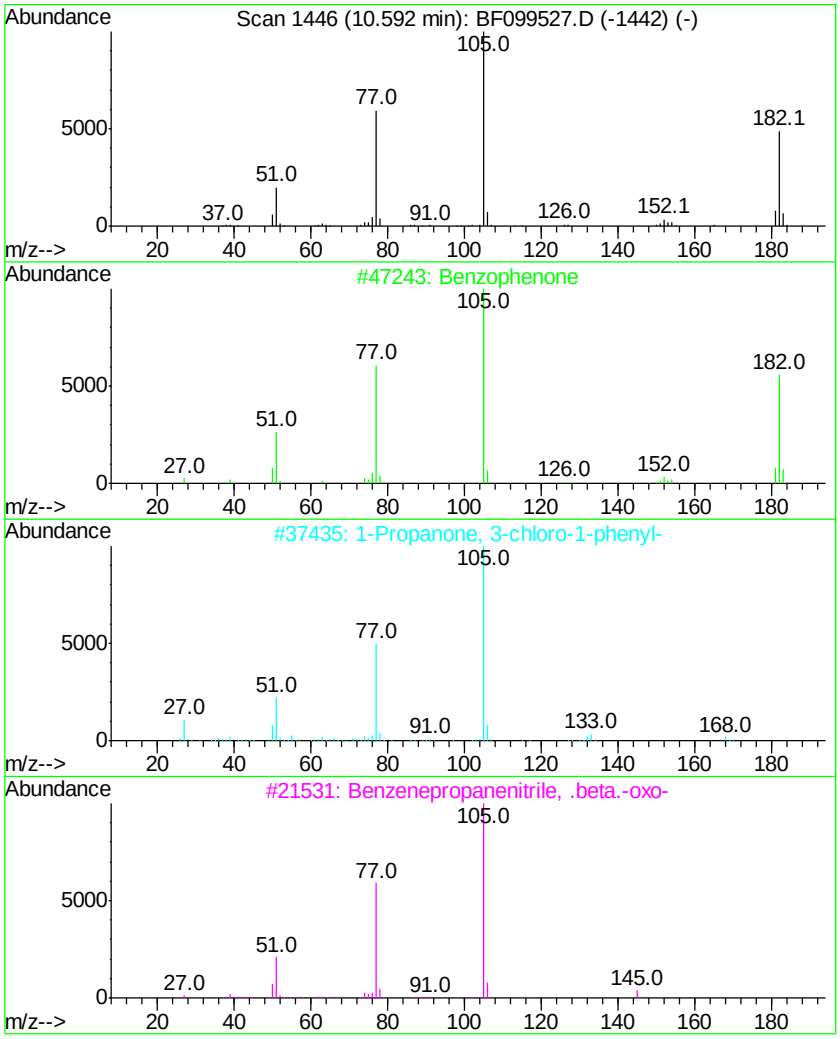
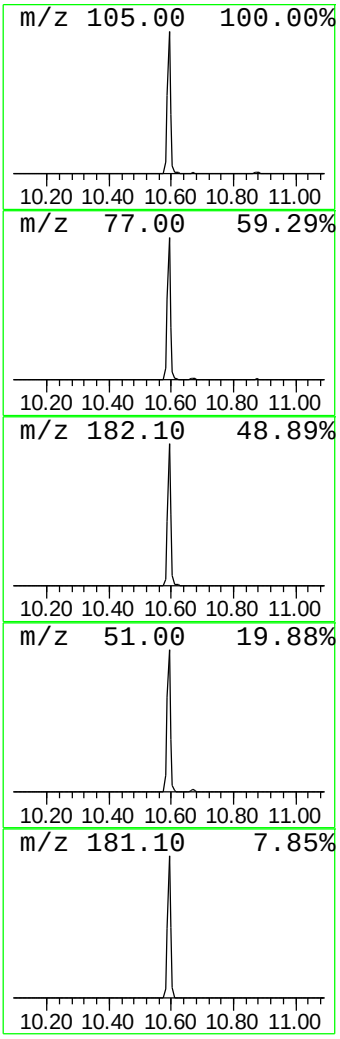
Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	14.12 ng	346774	Acenaphthene-d10	9.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	47
4	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47





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Sample : I5821-04
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WPSB-6B-18-18.5-BGS

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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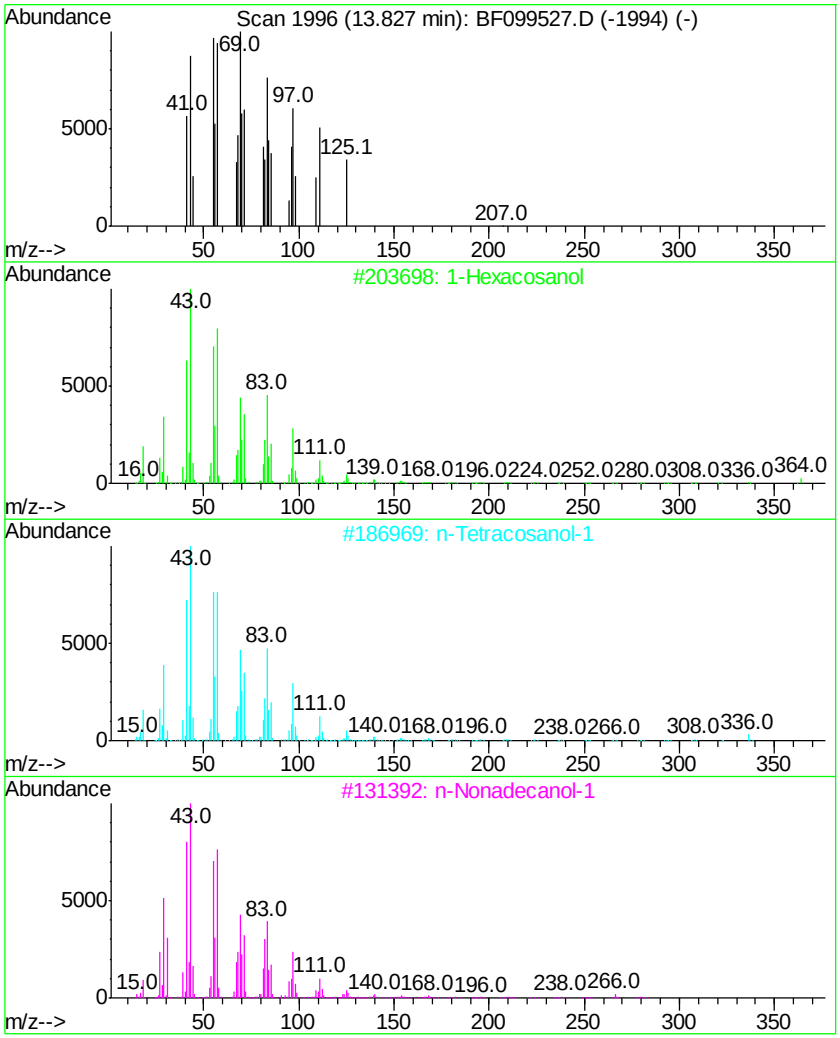
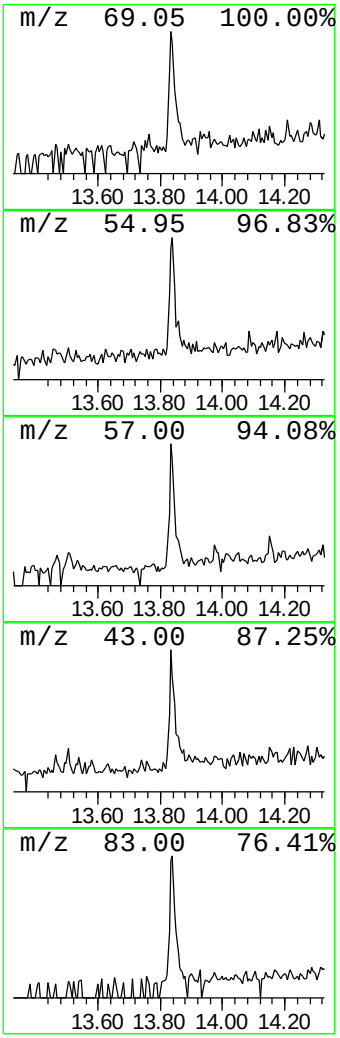
Peak Number 6 1-Hexacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	2.10 ng	47409	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	83
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	72
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	59
4	1-Eicosanol	298	C20H42O	000629-96-9	59
5	Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	47





Tentatively Identified Compound (LSC) summary

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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...	5.07	14.0	ng	315183	1	6.85	450068	20.0
unknown6.62	6.62	81.0	ng	1822060	1	6.85	450068	20.0
2-Hydroxy-iso-but...	8.68	4.0	ng	110249	2	8.13	551700	20.0
Benzophenone	10.59	14.1	ng	346774	3	9.88	491290	20.0
1-Hexacosanol	13.83	2.1	ng	47409	5	14.01	450975	20.0