LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
Data File : BF099947.D
Acq On : 29 Oct 2017 6:59
Operator : SJ/JU
Sample : I6100-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-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	4.998	493	495	510	rBV	84352	122636	3.67%	0.639%
2	5.410	562	565	591	rBV	660879	858362	25.69%	4.473%
3	6.428	736	738	755	rBV	448441	591716	17.71%	3.084%
4	6.557	757	760	767	rVB	1762532	1606828	48.09%	8.374%
5	6.787	795	799	808	rBV	705680	659579	19.74%	3.437%
6	6.939	821	825	841	rBV	2281175	2291077	68.57%	11.940%
7	7.357	892	896	899	rBV	1573191	1686783	50.48%	8.790%
8	8.069	1013	1017	1020	rBV	996399	907758	27.17%	4.731%
9	8.628	1109	1112	1121	rBV	111048	98313	2.94%	0.512%
10	9.145	1194	1200	1203	rBV	3286839	3341451	100.00%	17.413%
11	9.539	1264	1267	1276	rVB	148413	115577	3.46%	0.602%
12	9.822	1307	1315	1319	rBV	1068728	994896	29.77%	5.185%
13	9.857	1319	1321	1327	rVB	46518	40936	1.23%	0.213%
14	10.375	1406	1409	1416	rVB	36916	33873	1.01%	0.177%
15	10.492	1426	1429	1433	rBV	153607	123174	3.69%	0.642%
16	10.533	1433	1436	1442	rVV	439147	358938	10.74%	1.871%
17	10.616	1447	1450	1462	rBV	1085487	984656	29.47%	5.131%
18	11.316	1565	1569	1571	rBV	816180	773954	23.16%	4.033%
19	11.339	1571	1573	1578	rVB	90127	80218	2.40%	0.418%
20	12.698	1801	1804	1808	rVB	116790	103567	3.10%	0.540%
21	12.774	1814	1817	1821	rVB2	52635	49799	1.49%	0.260%
22	12.898	1833	1838	1841	rBV	2287998	2121396	63.49%	11.055%
23	13.404	1921	1924	1928	rVB	88448	71290	2.13%	0.372%
24	13.774	1984	1987	1997	rBV	74864	83423	2.50%	0.435%
25	13.963	2015	2019	2028	rBV	620642	567700	16.99%	2.958%
26	15.421	2263	2267	2276	rVB	395033	521057	15.59%	2.715%

Sum of corrected areas: 19188957

LSC Report - Integrated Chromatogram

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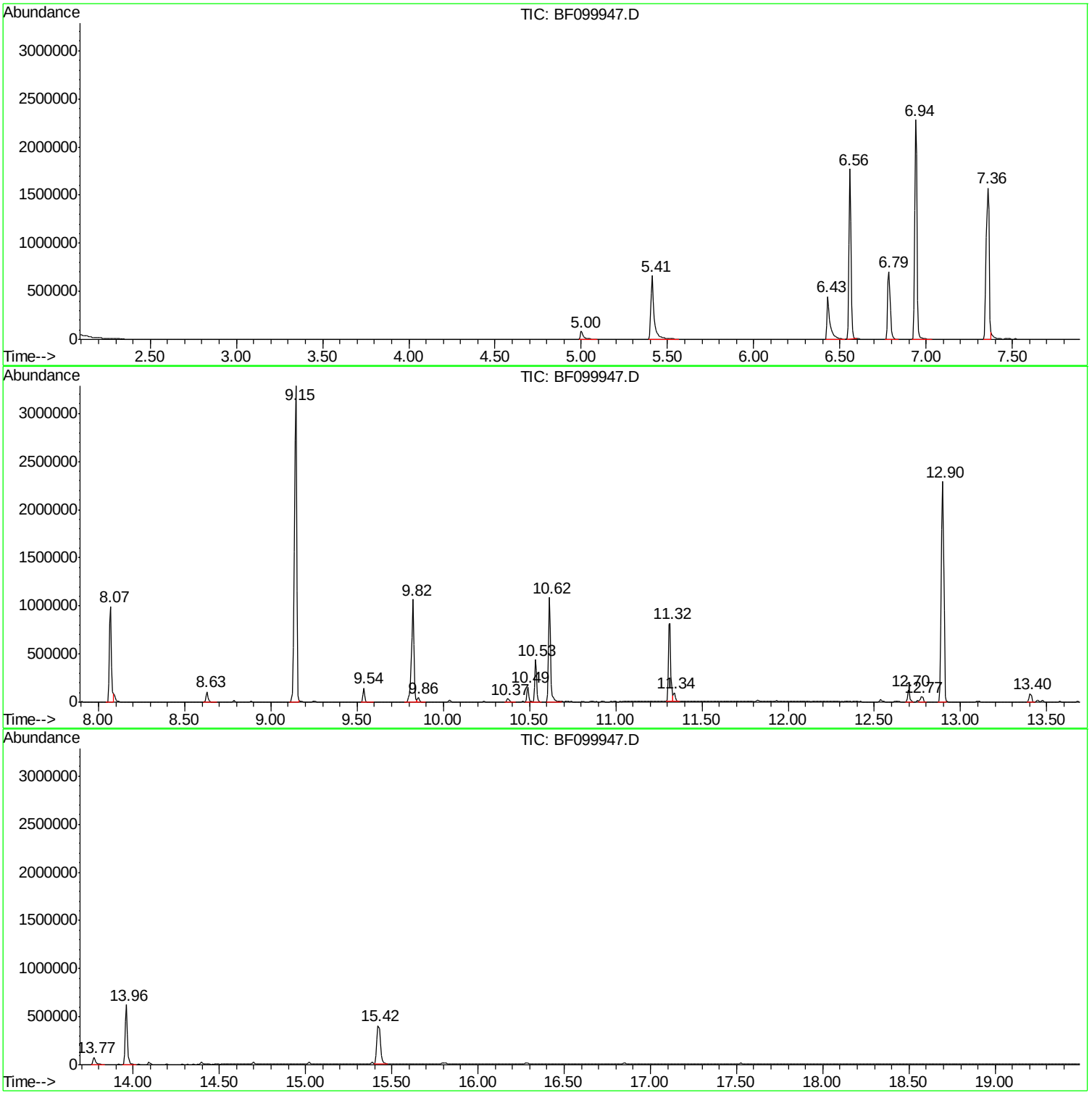
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF102817\
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Operator : SJ/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-S

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

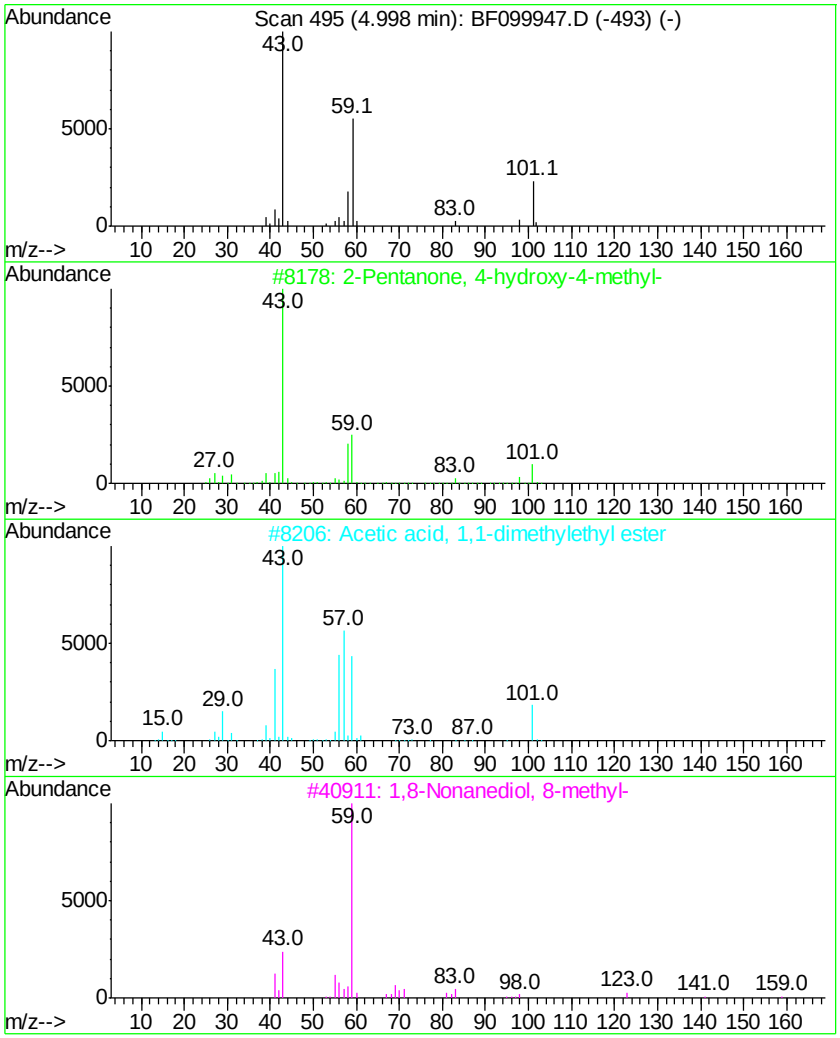
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

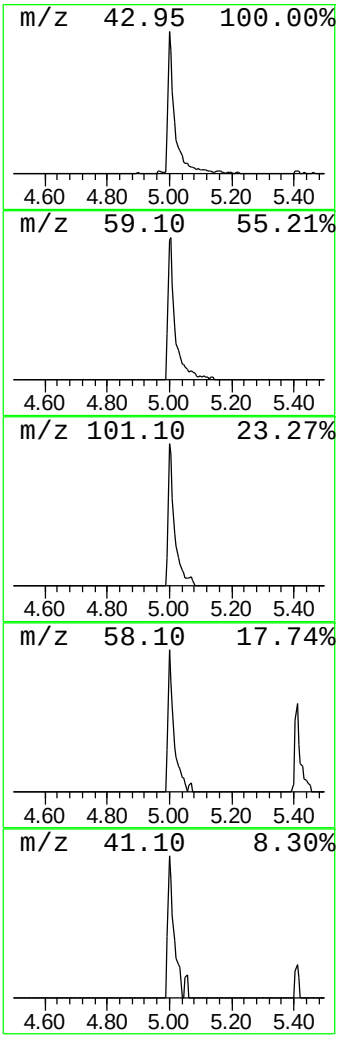
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.00	3.72 ng	122636	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	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : SJ/JU
Sample : I6100-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-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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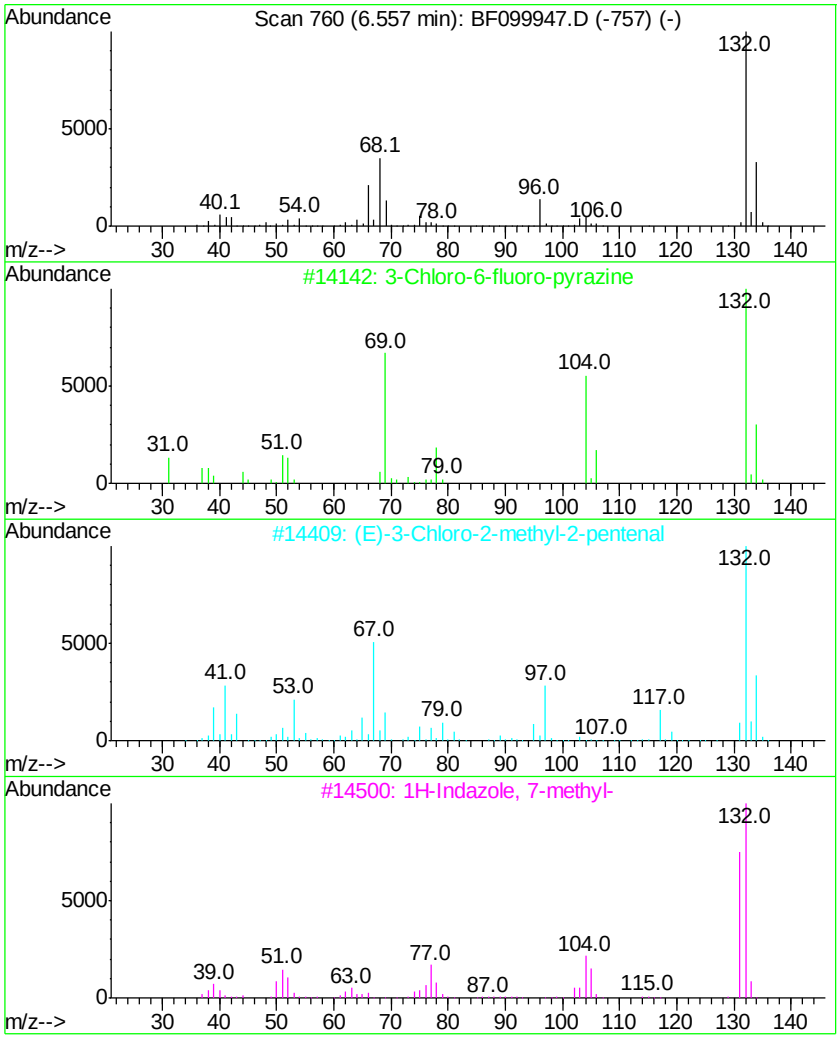
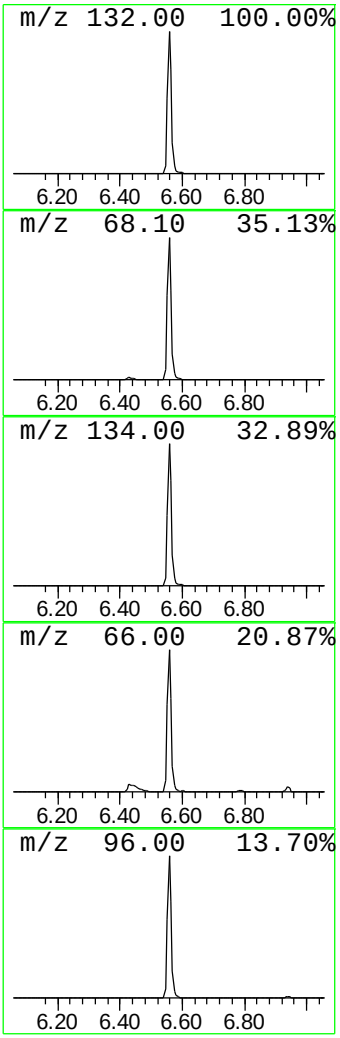
Peak Number 2 unknown6.56 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	48.72 ng	1606830	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	35
3	1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Operator : SJ/JU
Sample : I6100-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-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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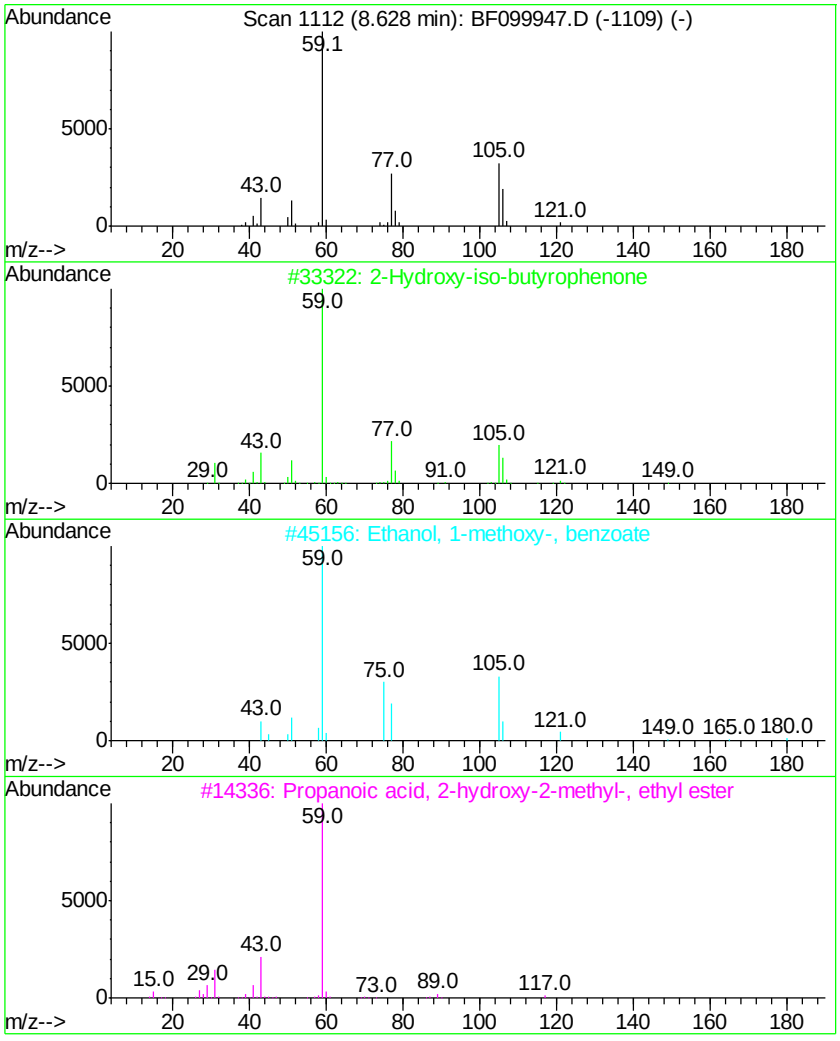
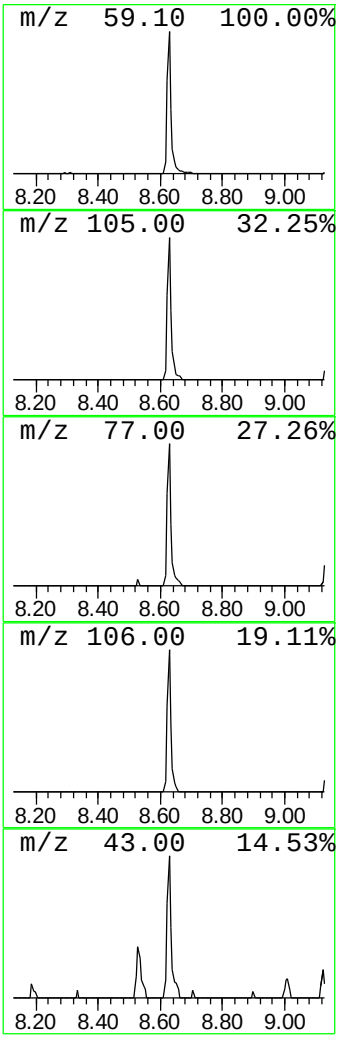
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	2.17 ng	98313	Naphthalene-d8	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
4	Guanidine	59	CH5N3	000113-00-8	7
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5





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Data File : BF099947.D
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Operator : SJ/JU
Sample : I6100-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

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

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

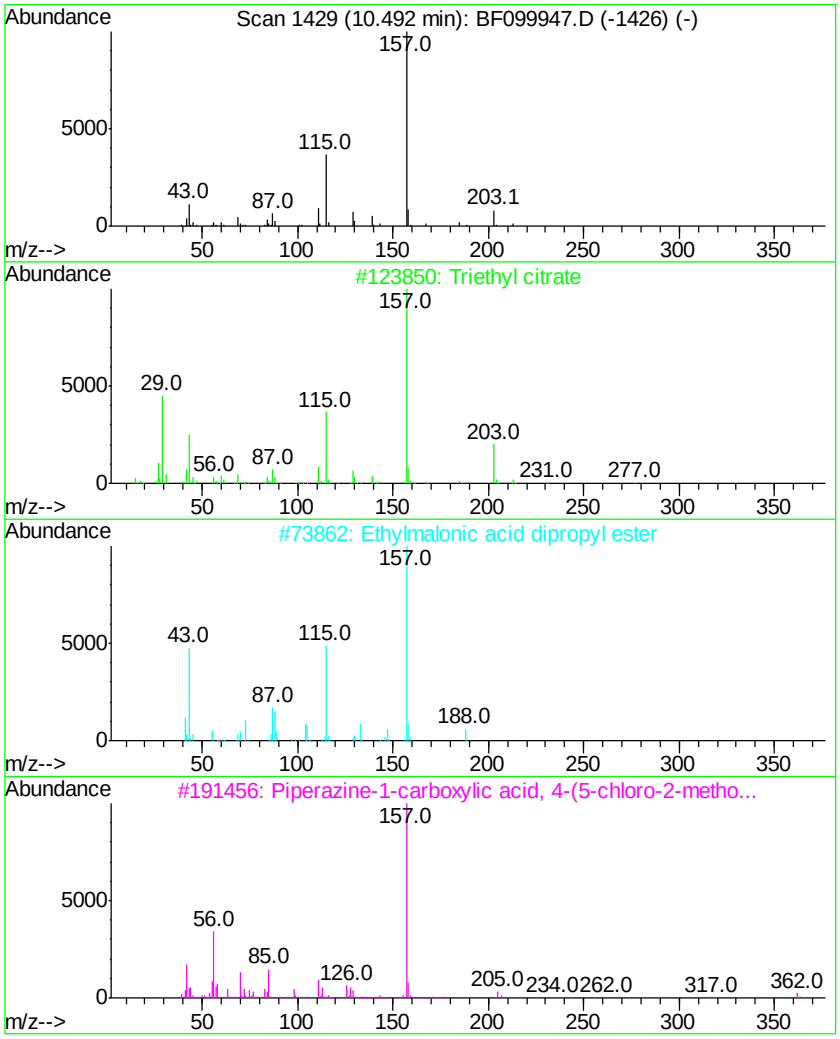
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

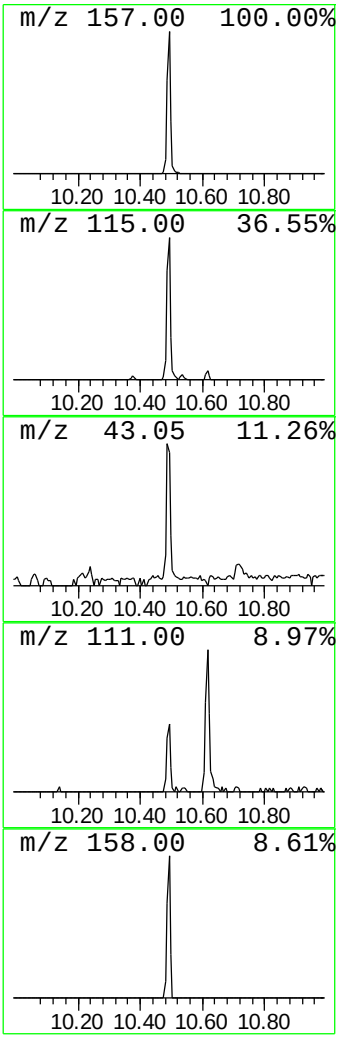
****

Peak Number 5 Triethyl citrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.49	2.48 ng	123174	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethyl citrate	276	C12H20O7	000077-93-0	53
2	Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	39
3	Piperazine-1-carboxylic acid, 4-...	362	C14H19ClN2O5S	1000303-80-2	36
4	Piperazine-1-carboxylic acid, 4-...	396	C14H18Cl2N2O5S	1000303-80-3	36
5	3-Chloro2-fluorobenzoic acid, 3-...	370	C21H32ClFO2	1000338-64-6	36





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Data File : BF099947.D
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Operator : SJ/JU
Sample : I6100-02
Misc :
ALS Vial : 37 Sample Multiplier: 1

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

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

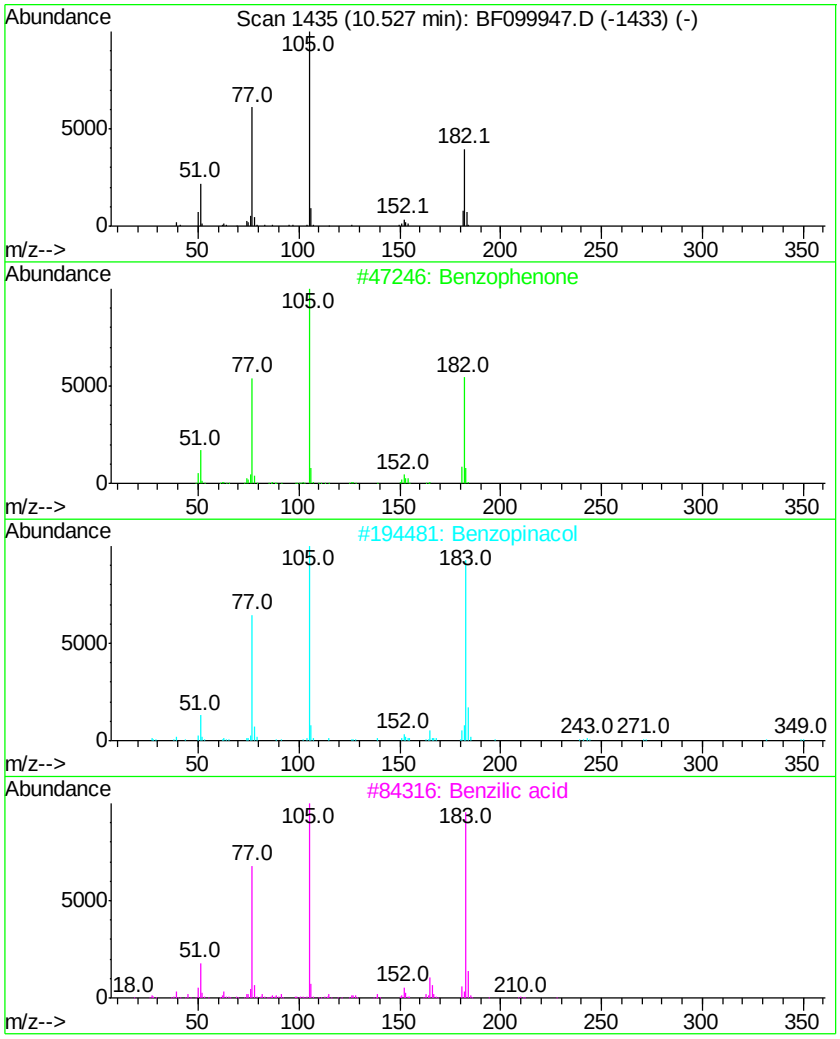
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

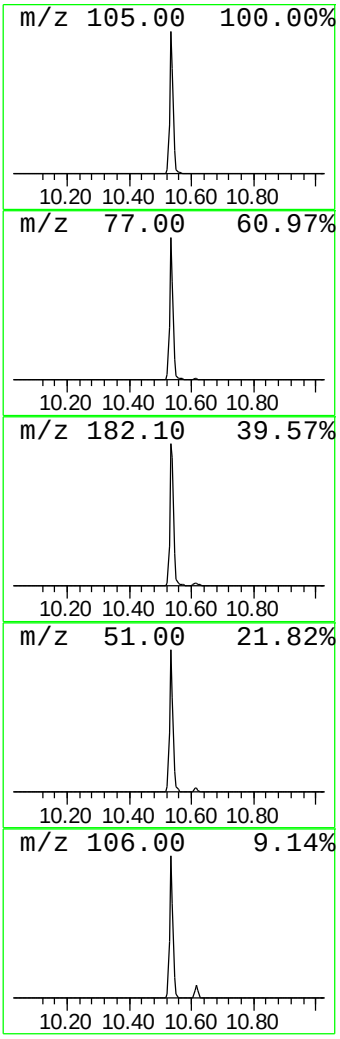
****

Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.53	7.22 ng	358938	Acenaphthene-d10	9.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzopinacol	366	C26H22O2	000464-72-2	50
3	Benzilic acid	228	C14H12O3	000076-93-7	50
4	Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
5	Methyl benzilate	242	C15H14O3	000076-89-1	47





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ALS Vial : 37 Sample Multiplier: 1

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

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

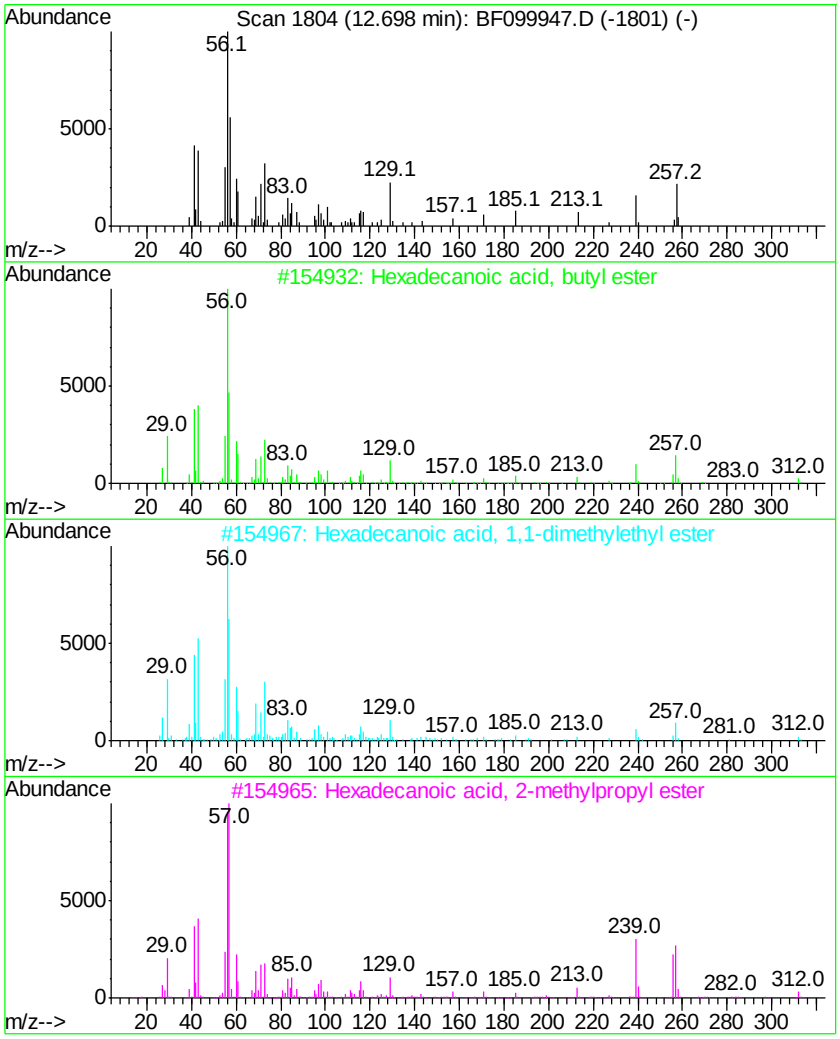
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

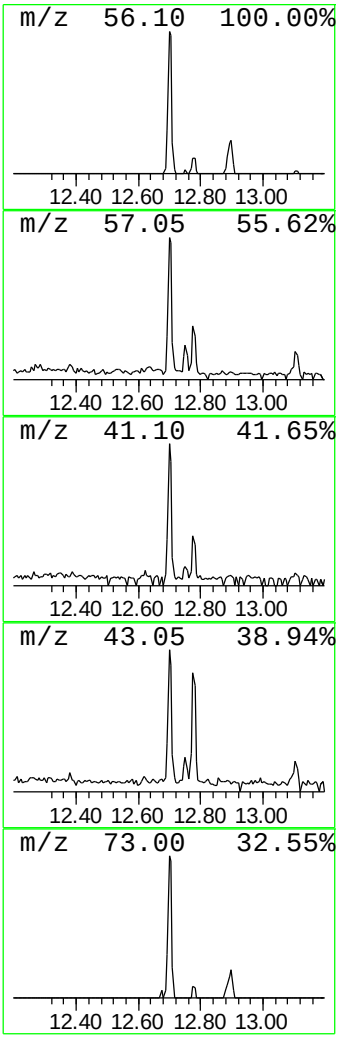
****

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	3.65 ng	103567	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	53
4	Nipecotic acid	129	C6H11NO2	000498-95-3	47
5	3-Amino-2,2-dimethyl-1-propanol	103	C5H13NO	026734-09-8	35





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Misc :
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Instrument : BNA_F
ClientSampleId : 102317-TIDO-F-D-S

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

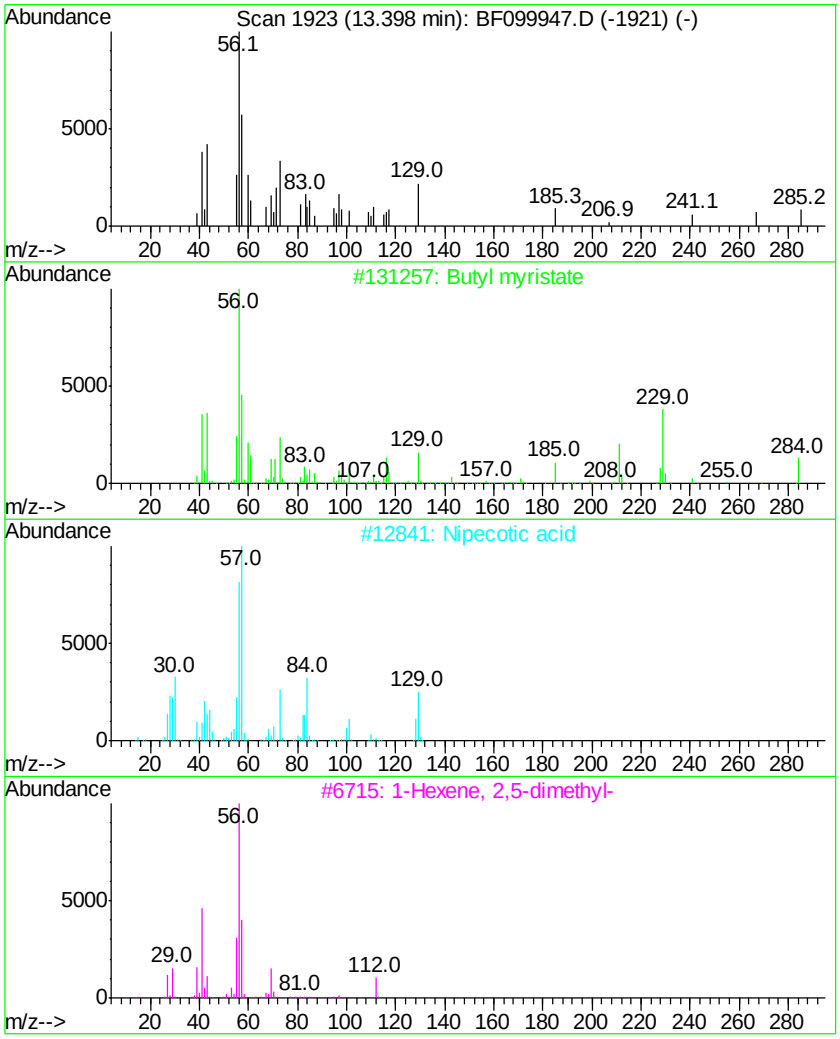
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

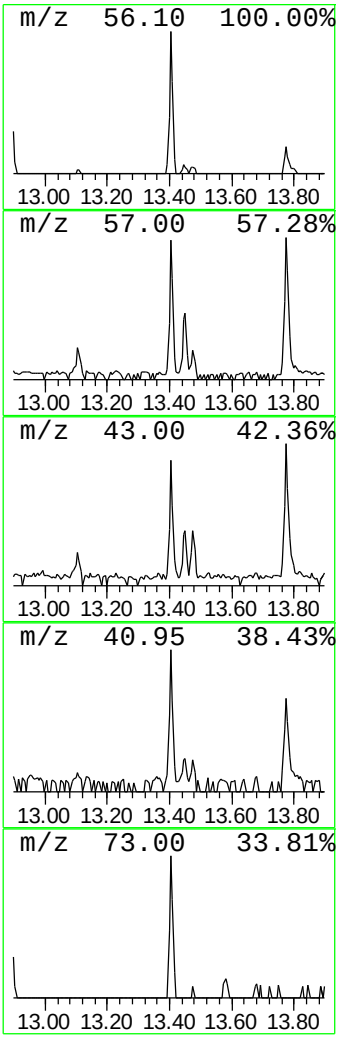
****

Peak Number 8 Butyl myristate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.51 ng	71290	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	64
2	Nipecotic acid	129	C6H11NO2	000498-95-3	38
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30
4	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	27
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27





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BNA_F
ClientSampleId :
102317-TIDO-F-D-S

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF102317.M
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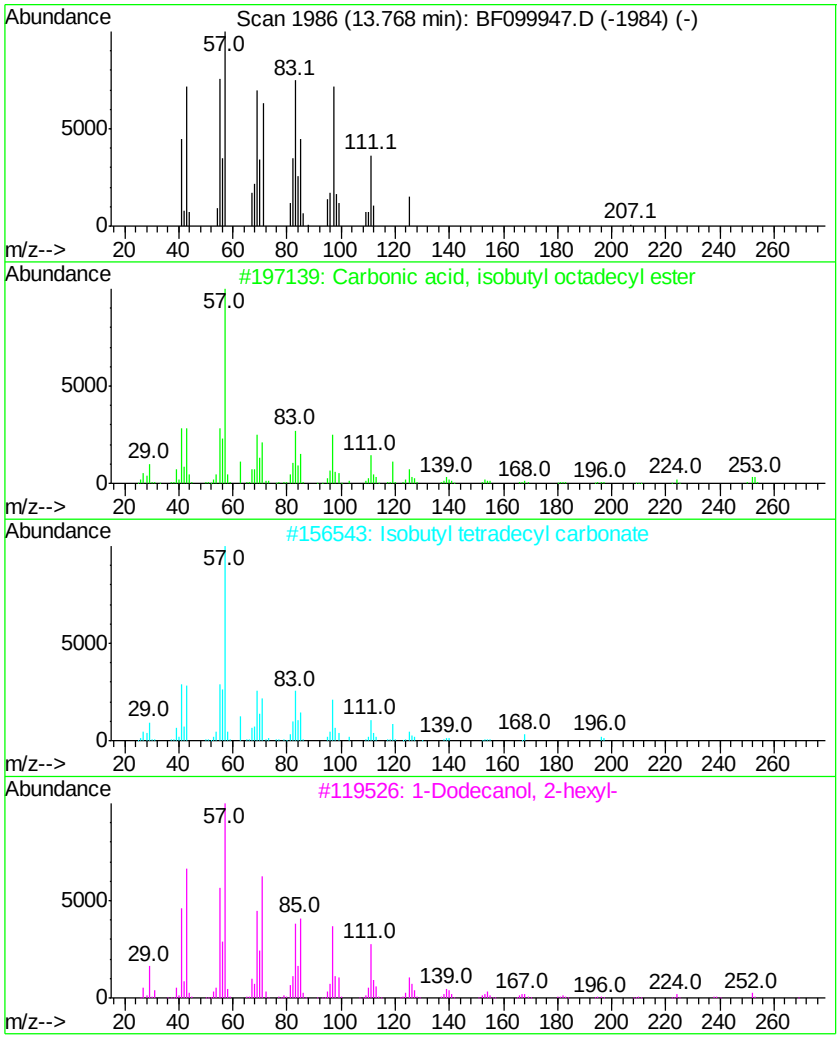
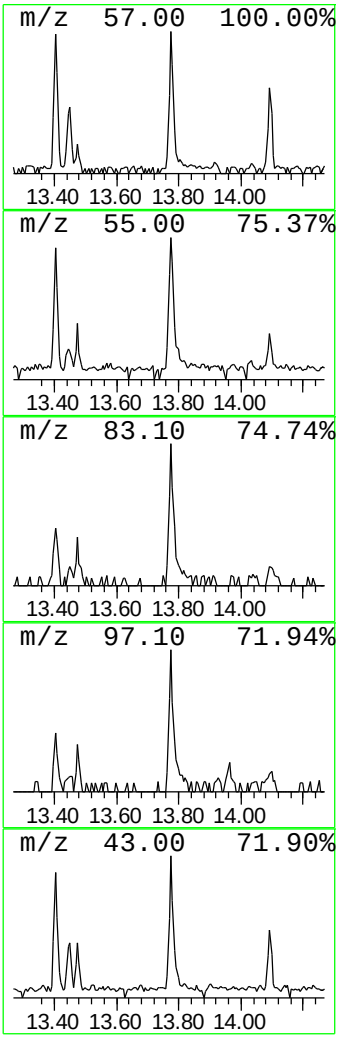
****

Peak Number 9 Carbonic acid, isobutyl oct... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.77	2.94 ng	83423	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	90
2	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	90
3	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	76
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	76
5	17-Pentatriacontene	491	C35H70	006971-40-0	74





Tentatively Identified Compound (LSC) summary

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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	3.7	ng	122636	1	6.79	659579	20.0
unknown6.56	6.56	48.7	ng	1606830	1	6.79	659579	20.0
2-Hydroxy-iso-but...	8.63	2.2	ng	98313	2	8.07	907758	20.0
Triethyl citrate	10.49	2.5	ng	123174	3	9.82	994896	20.0
Benzophenone	10.53	7.2	ng	358938	3	9.82	994896	20.0
Hexadecanoic acid...	12.70	3.6	ng	103567	5	13.96	567700	20.0
Butyl myristate	13.40	2.5	ng	71290	5	13.96	567700	20.0
Carbonic acid, is...	13.77	2.9	ng	83423	5	13.96	567700	20.0