LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100360.D
Acq On : 10 Nov 2017 00:11
Operator : SJ/JU
Sample : I6388-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-3

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-BF110817.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	2.228	22	24	42	rVB3	46591	114682	2.88%	0.321%
2	5.140	514	519	529	rVB	638521	866379	21.73%	2.429%
3	5.528	579	585	588	rBV	3454038	3752036	94.08%	10.518%
4	6.528	748	755	759	rBV	3510851	3987931	100.00%	11.179%
5	6.675	774	780	783	rBV	3582852	3801647	95.33%	10.657%
6	6.904	815	819	822	rBV	1379550	1157712	29.03%	3.245%
7	7.057	841	845	849	rVB	2903567	2692062	67.51%	7.547%
8	7.463	909	914	917	rBV	2502296	2449345	61.42%	6.866%
9	8.181	1032	1036	1040	rBV	1621845	1495212	37.49%	4.191%
10	8.734	1126	1130	1134	rBV	461006	379458	9.52%	1.064%
11	9.257	1214	1219	1222	rBV	3771285	3393989	85.11%	9.514%
12	9.645	1282	1285	1289	rBV	674821	568018	14.24%	1.592%
13	9.939	1330	1335	1339	rBV	1762661	1553136	38.95%	4.354%
14	10.651	1451	1456	1459	rBV	1492391	1160333	29.10%	3.253%
15	10.728	1464	1469	1472	rBV	2007106	1897691	47.59%	5.320%
16	11.422	1582	1587	1591	rBV	1487184	1359257	34.08%	3.810%
17	11.939	1669	1675	1686	rBV	338774	352245	8.83%	0.987%
18	12.727	1805	1809	1819	rBV	128979	156993	3.94%	0.440%
19	13.004	1852	1856	1860	rBV	2045831	1902396	47.70%	5.333%
20	13.892	2004	2007	2017	rBV	460663	453319	11.37%	1.271%
21	14.063	2032	2036	2039	rVB	1123427	999324	25.06%	2.801%
22	14.527	2112	2115	2119	rBV5	39072	46778	1.17%	0.131%
23	15.545	2283	2288	2298	rVB	834914	1080682	27.10%	3.029%
24	16.062	2373	2376	2381	rVB5	41279	52297	1.31%	0.147%

Sum of corrected areas: 35672922

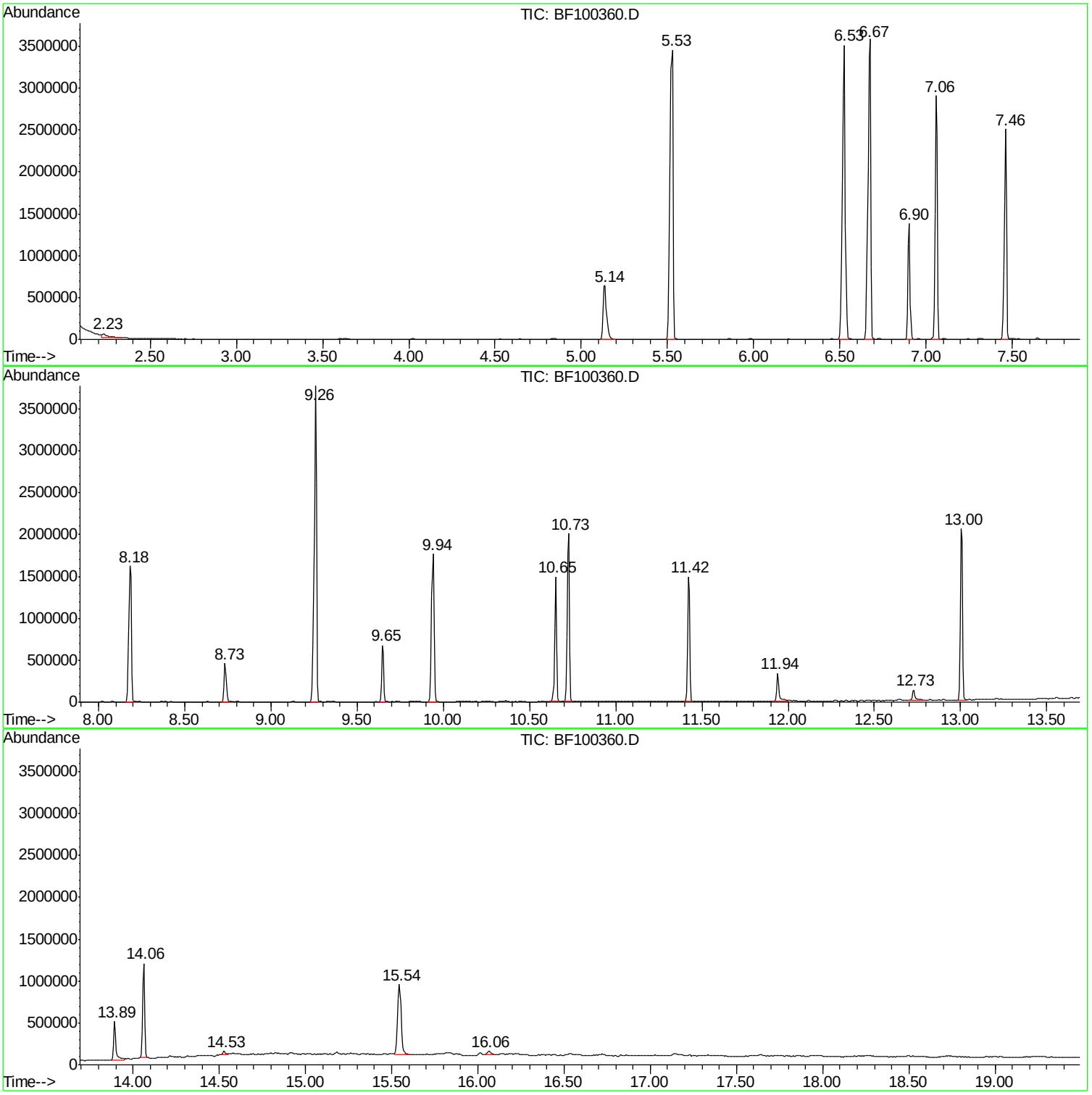
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100360.D
Acq On : 10 Nov 2017 00:11
Operator : SJ/JU
Sample : I6388-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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\BF110917\
Data File : BF100360.D
Acq On : 10 Nov 2017 00:11
Operator : SJ/JU
Sample : I6388-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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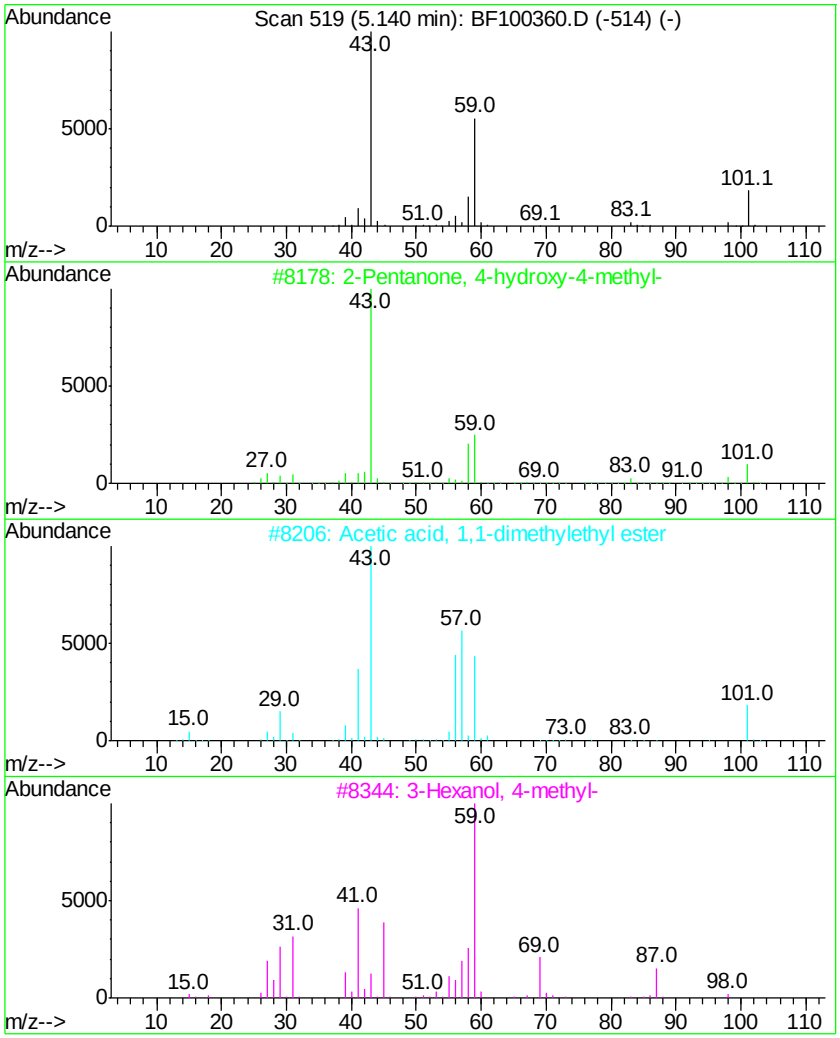
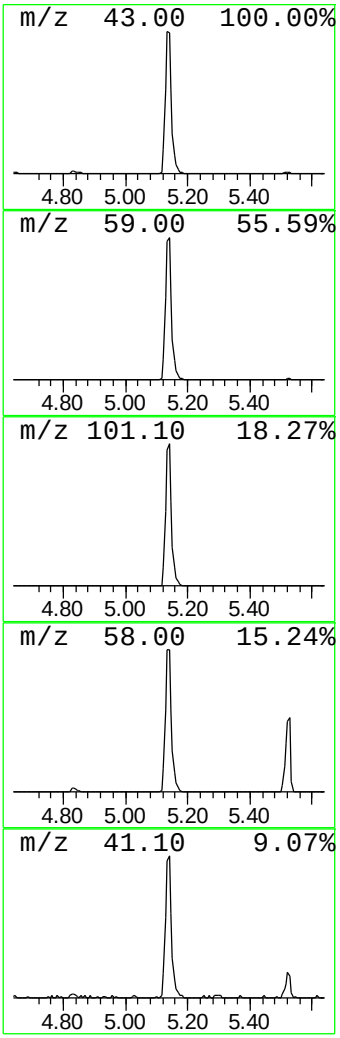
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	14.97 ng	866379	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100360.D
Acq On : 10 Nov 2017 00:11
Operator : SJ/JU
Sample : I6388-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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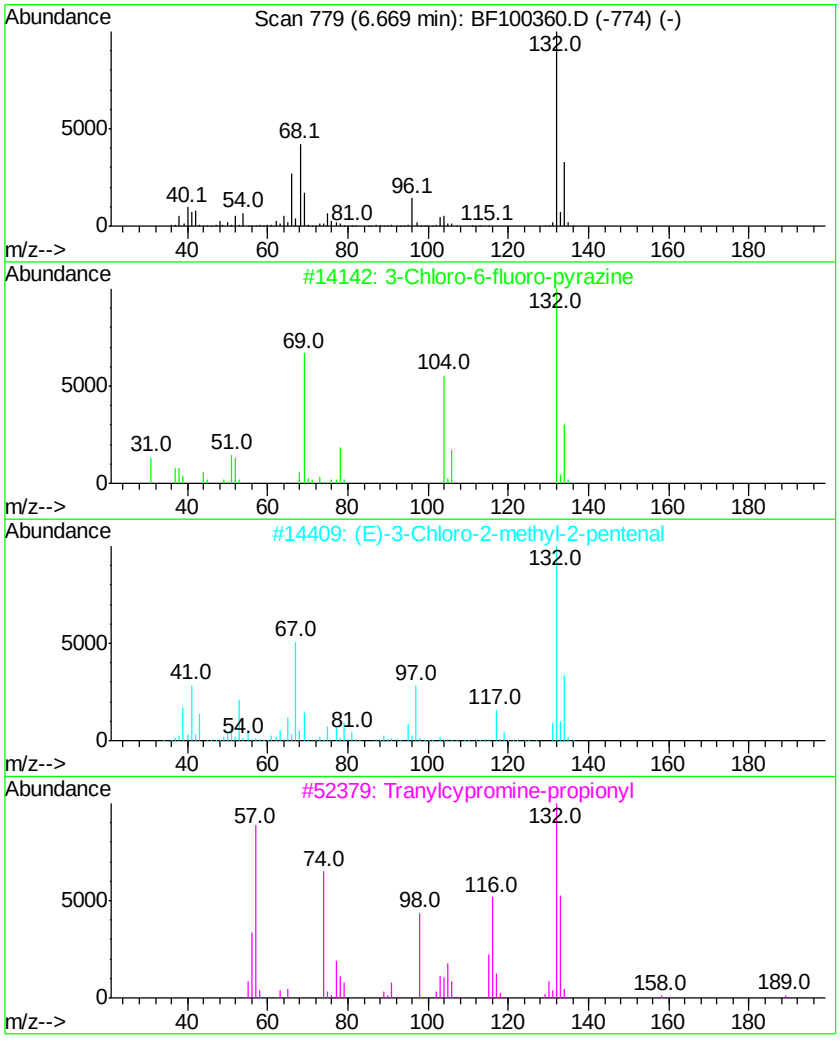
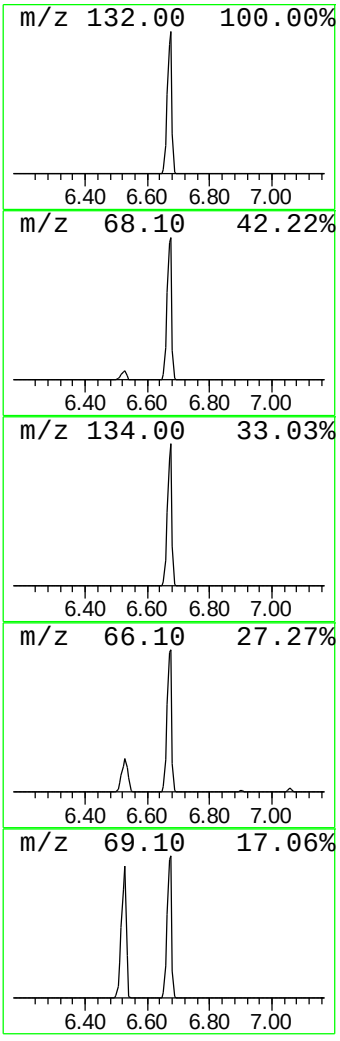
Peak Number 2 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	65.68 ng	3801650	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Data File : BF100360.D
Acq On : 10 Nov 2017 00:11
Operator : SJ/JU
Sample : I6388-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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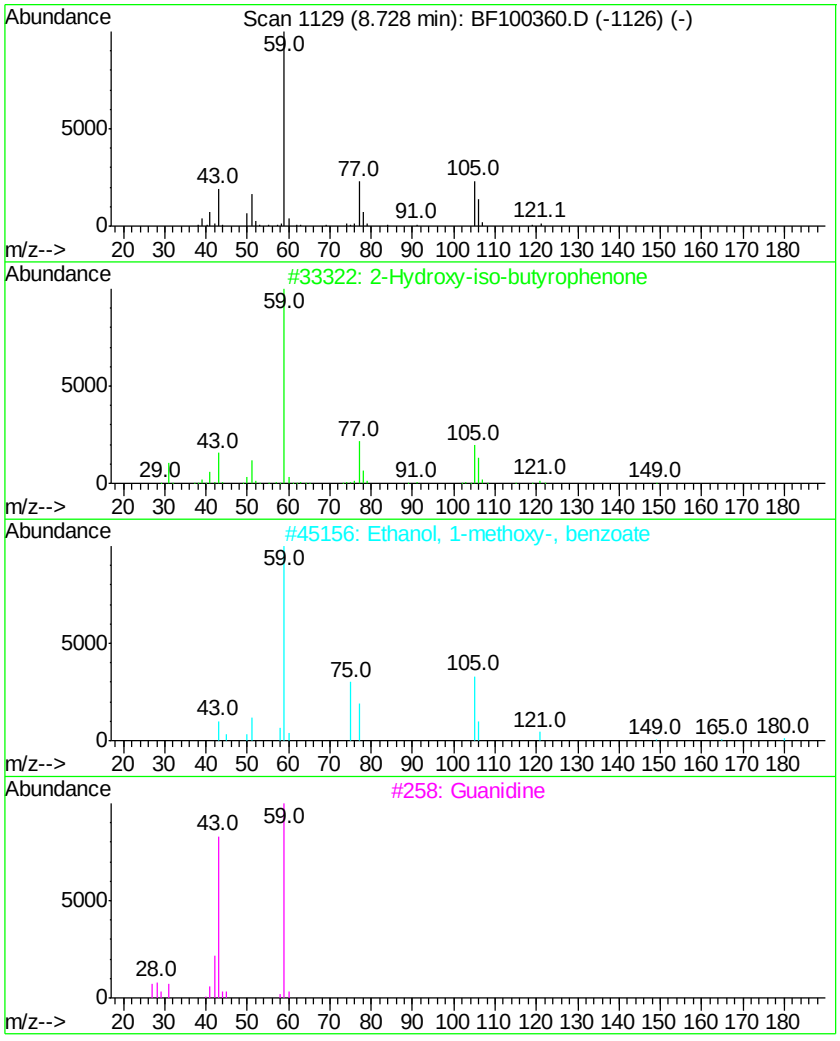
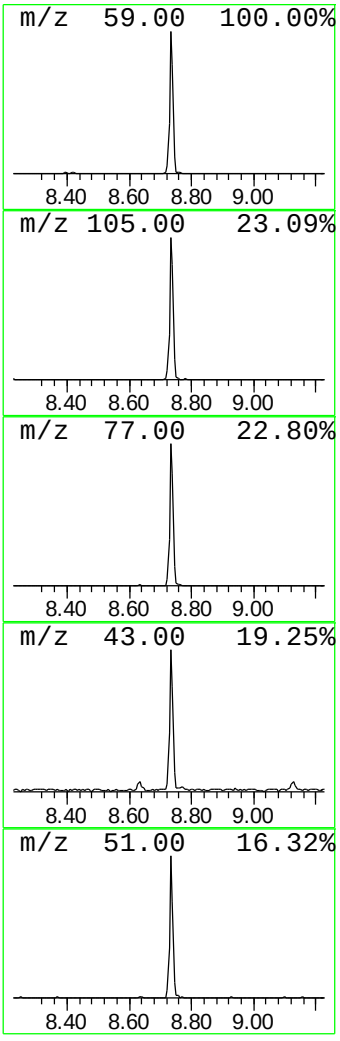
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	5.08 ng	379458	Naphthalene-d8	8.18

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	Guanidine	59	CH5N3	000113-00-8	7
4	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
5	Acetamide	59	C2H5NO	000060-35-5	5





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF110917\
Data File : BF100360.D
Acq On : 10 Nov 2017 00:11
Operator : SJ/JU
Sample : I6388-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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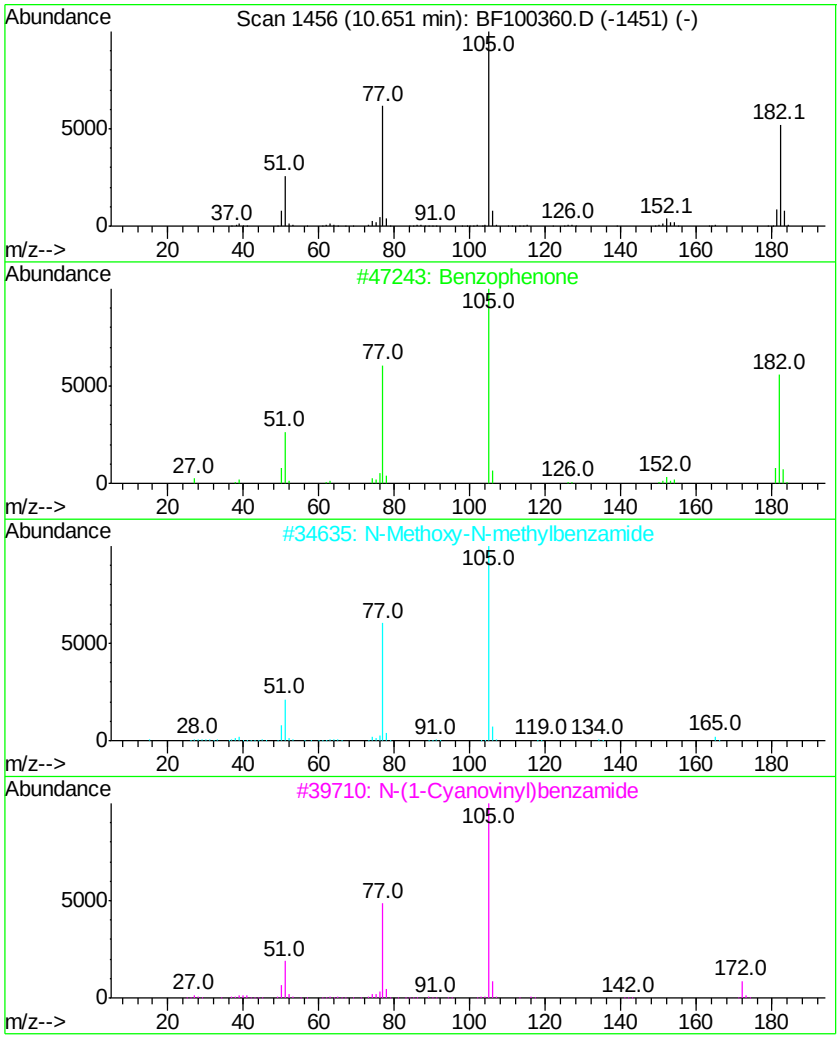
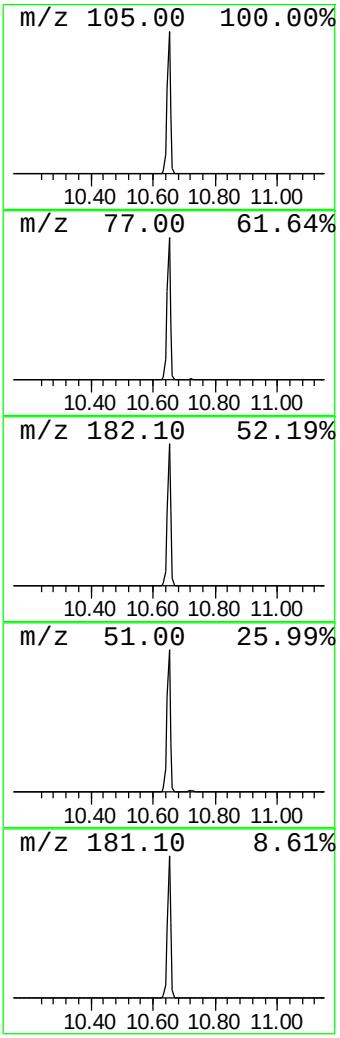
Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	14.94 ng	1160330	Acenaphthene-d10	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47
3	N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47
4	Vinyl benzoate	148	C9H8O2	000769-78-8	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





Library Search Compound Report

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Sample : I6388-05
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-3

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

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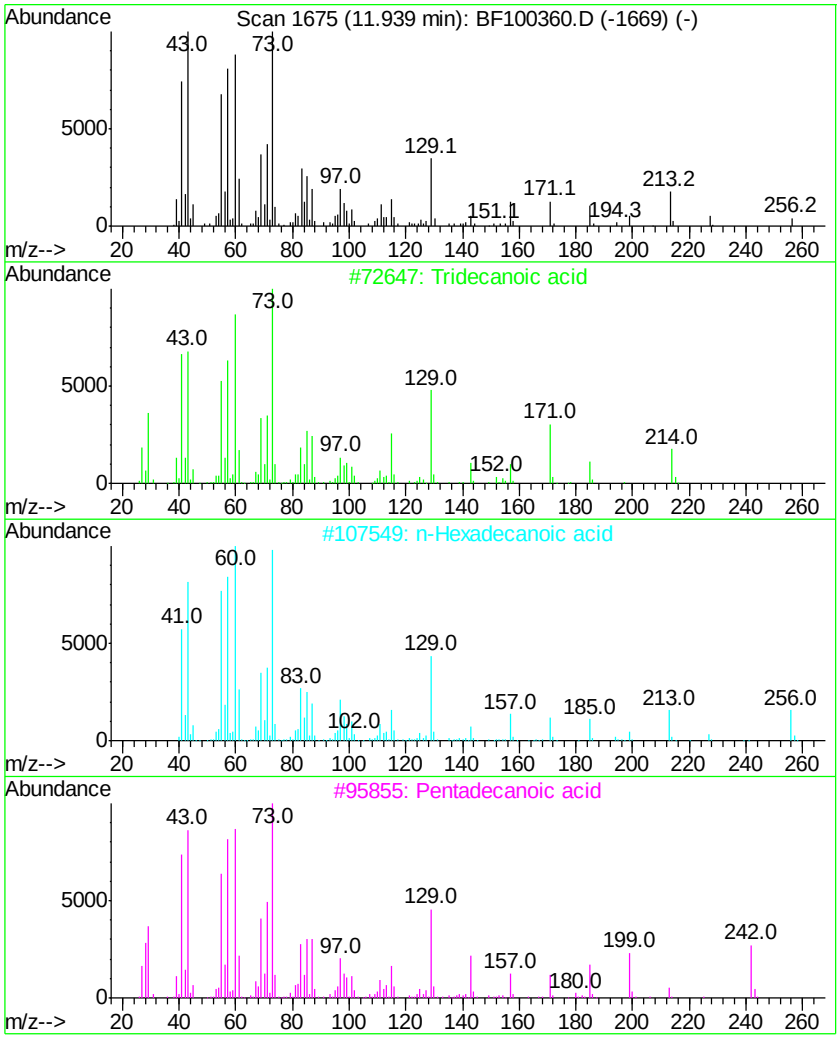
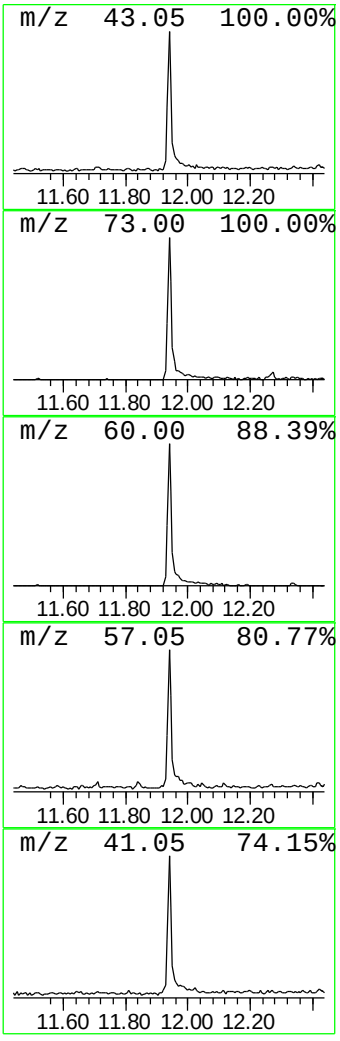
Peak Number 6 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	5.18 ng	352245	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	n-Decanoic acid	172	C10H20O2	000334-48-5	25





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Misc :
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Instrument : BNA_F
ClientSampleId : 3N-3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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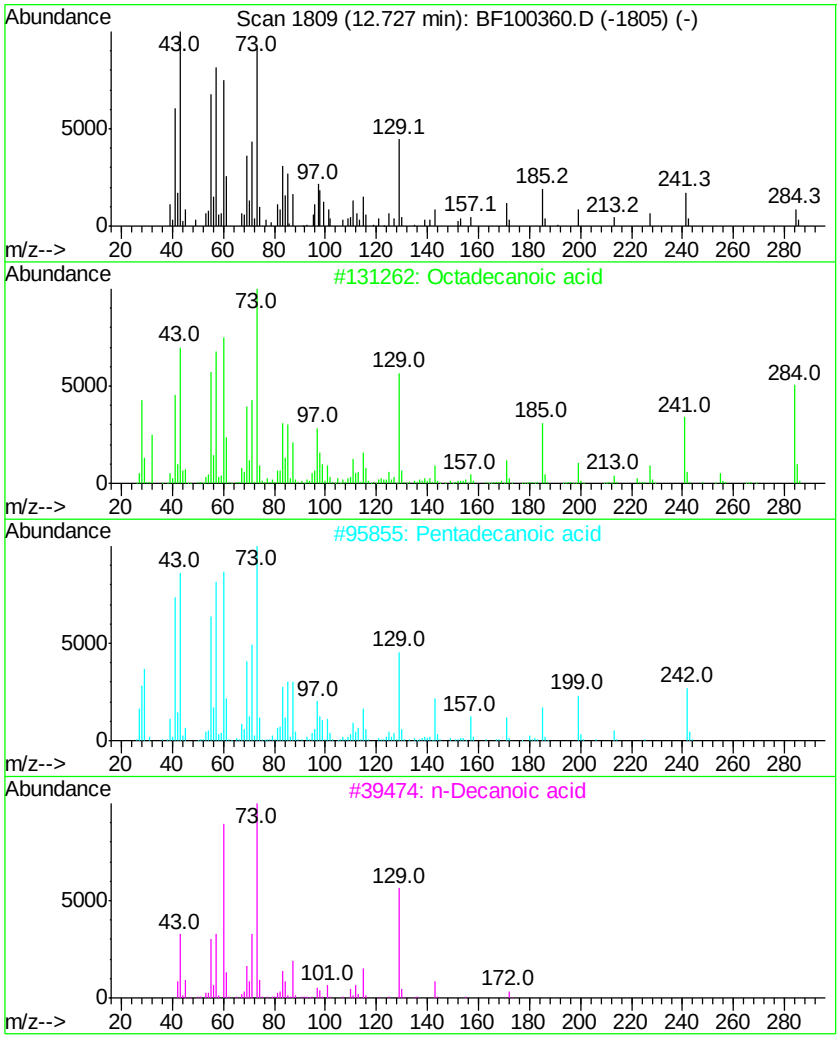
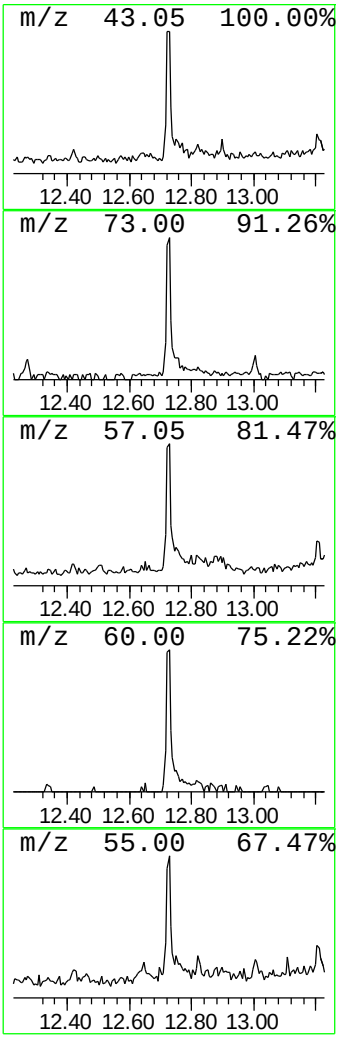
Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	2.31 ng	156993	Phenanthrene-d10	11.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Decanoic acid	172	C10H20O2	000334-48-5	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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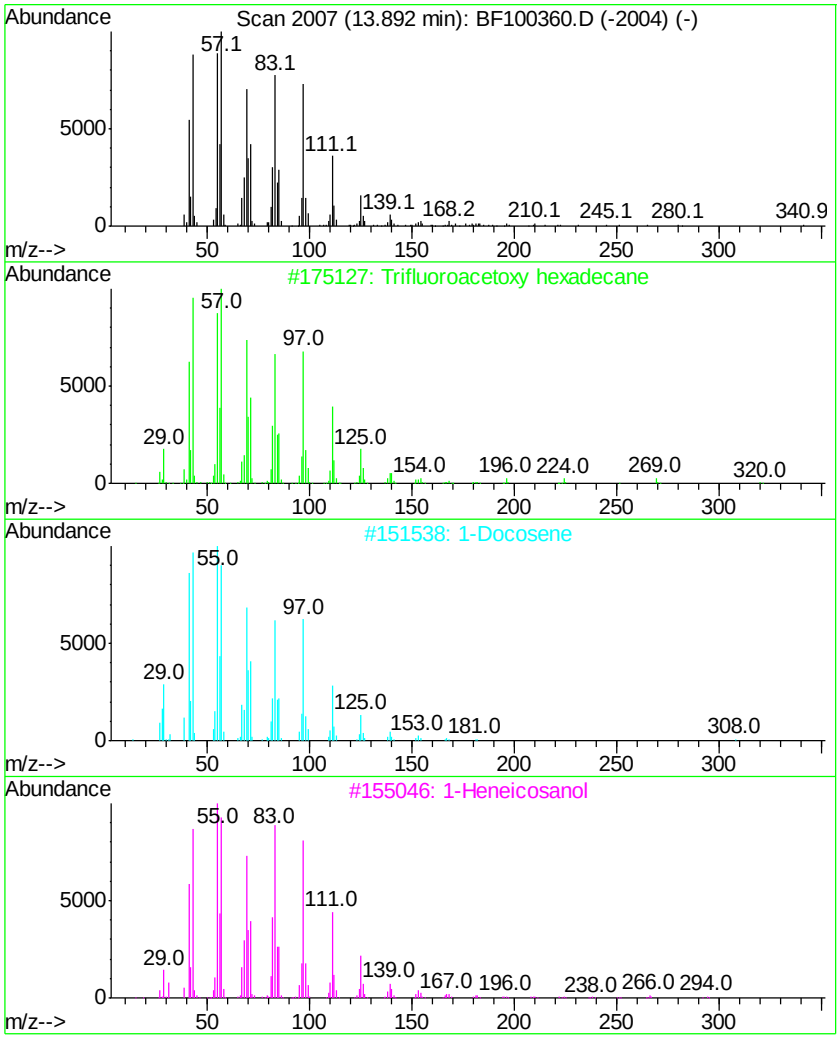
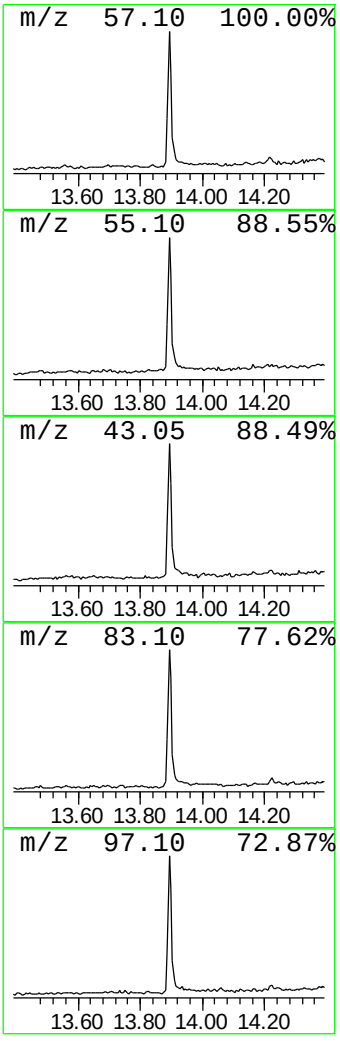
Peak Number 8 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	9.07 ng	453319	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Behenic alcohol	326	C22H46O	000661-19-8	93
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	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
2-Pentanone, 4-hy...	5.14	15.0	ng	866379	1	6.90	1157710	20.0
unknown6.67	6.67	65.7	ng	3801650	1	6.90	1157710	20.0
2-Hydroxy-iso-but...	8.73	5.1	ng	379458	2	8.18	1495210	20.0
Benzophenone	10.65	14.9	ng	1160330	3	9.94	1553140	20.0
Tridecanoic acid	11.94	5.2	ng	352245	4	11.42	1359260	20.0
Octadecanoic acid	12.73	2.3	ng	156993	4	11.42	1359260	20.0
Trifluoroacetoxy ...	13.89	9.1	ng	453319	5	14.06	999324	20.0