LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
Data File : BF107776.D
Acq On : 28 Jul 2018 5:36
Operator : JU/SJ
Sample : J4199-01
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-33

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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	5.190	482	485	496	rBV	160940	196314	4.22%	0.641%
2	5.596	551	554	578	rBV	854041	1516265	32.56%	4.951%
3	6.601	722	725	744	rBV	400670	1011666	21.72%	3.303%
4	6.737	744	748	769	rVV	2512273	3347906	71.89%	10.931%
5	6.960	783	786	793	rBV	513177	721891	15.50%	2.357%
6	7.119	809	813	836	rBV	2737985	3433353	73.73%	11.210%
7	7.531	879	883	900	rBV	1635755	2588945	55.59%	8.453%
8	7.737	916	918	932	rVB4	30619	67893	1.46%	0.222%
9	8.242	1000	1004	1021	rBV	843127	1111332	23.86%	3.629%
10	9.054	1136	1142	1149	rBV	82121	109399	2.35%	0.357%
11	9.319	1182	1187	1202	rBV	3723752	4656957	100.00%	15.206%
12	9.707	1248	1253	1261	rVV	166431	192059	4.12%	0.627%
13	9.772	1261	1264	1273	rVB4	24801	48483	1.04%	0.158%
14	9.901	1281	1286	1291	rBV	84471	102677	2.20%	0.335%
15	10.001	1299	1303	1306	rBV	1042349	990003	21.26%	3.232%
16	10.031	1306	1308	1318	rVB	199619	244977	5.26%	0.800%
17	10.795	1434	1438	1459	rBV	1985022	2647589	56.85%	8.645%
18	11.495	1553	1557	1569	rBV	806081	1071792	23.01%	3.500%
19	12.001	1640	1643	1647	rBV	76111	87343	1.88%	0.285%
20	12.125	1660	1664	1672	rBV2	90012	118270	2.54%	0.386%
21	13.083	1822	1827	1840	rBV	3346874	3965485	85.15%	12.948%
22	13.954	1972	1975	1980	rBV	107696	97110	2.09%	0.317%
23	14.148	2004	2008	2019	rBV	928844	1109350	23.82%	3.622%
24	14.577	2079	2081	2085	rVB2	43219	48446	1.04%	0.158%
25	14.895	2132	2135	2140	rBV	66930	68283	1.47%	0.223%
26	15.248	2192	2195	2201	rVB	81718	102020	2.19%	0.333%
27	15.683	2264	2269	2282	rVB	482333	854225	18.34%	2.789%
28	16.112	2338	2342	2347	rVB2	76949	116564	2.50%	0.381%

Sum of corrected areas: 30626597

LSC Report - Integrated Chromatogram

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Misc :
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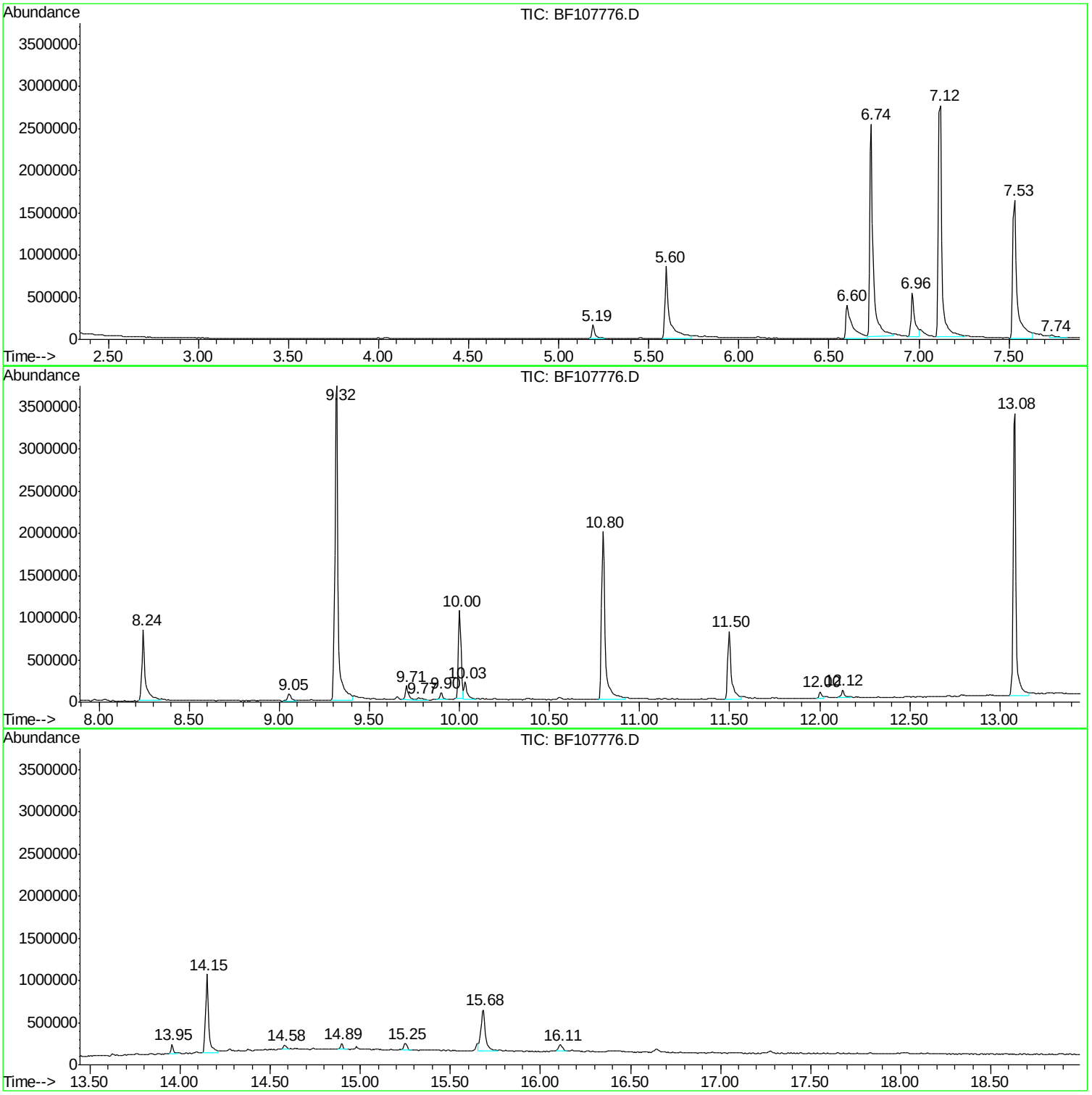
Instrument : BNA_F
ClientSampleId : MW-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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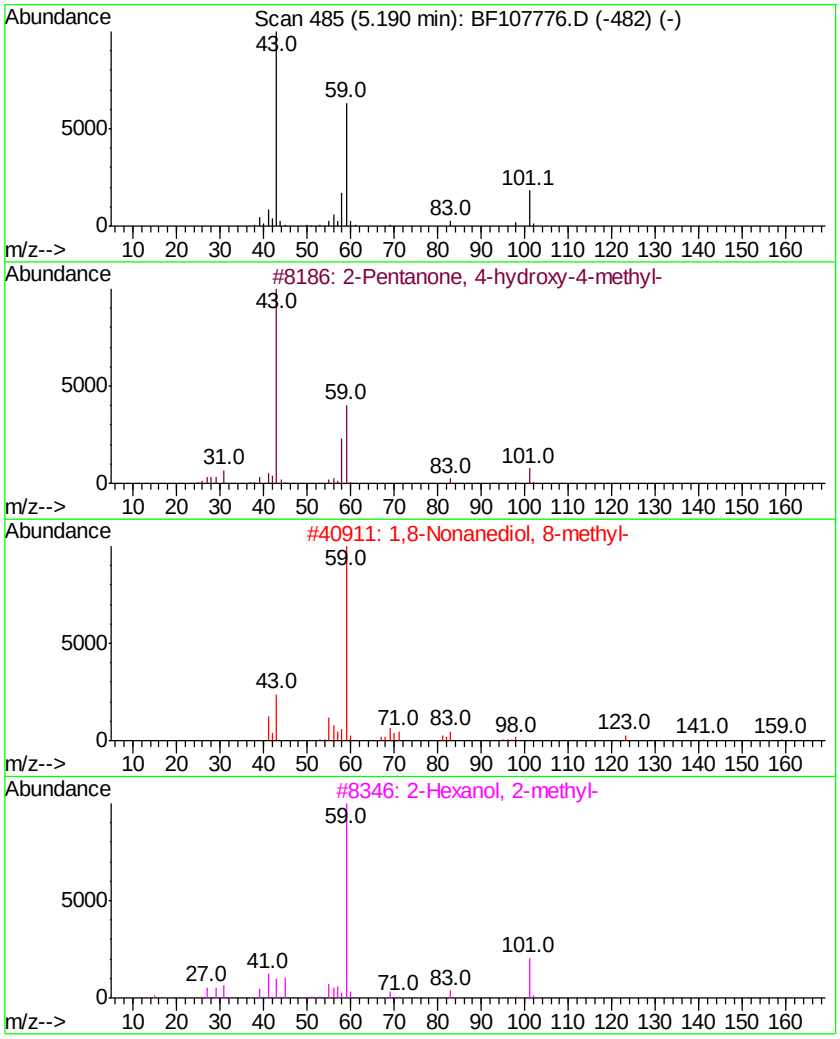
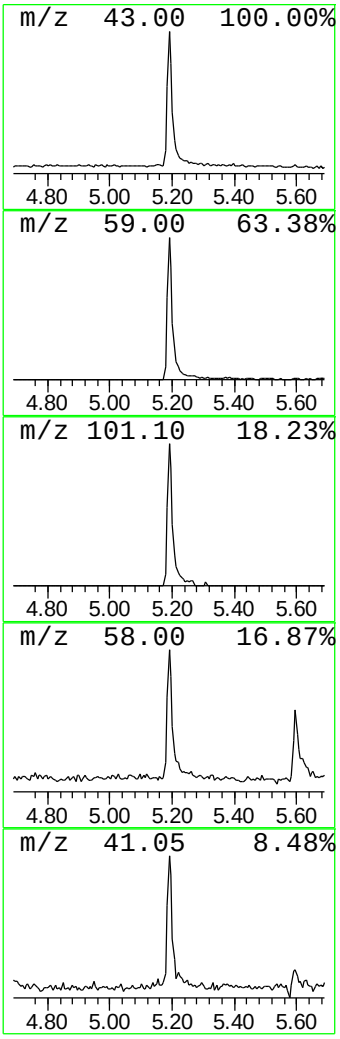
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	5.44 ng	196314	1,4-Dichlorobenzene-d4	6.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	38
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4	3-Octanol	130	C8H18O	000589-98-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





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Operator : JU/SJ
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Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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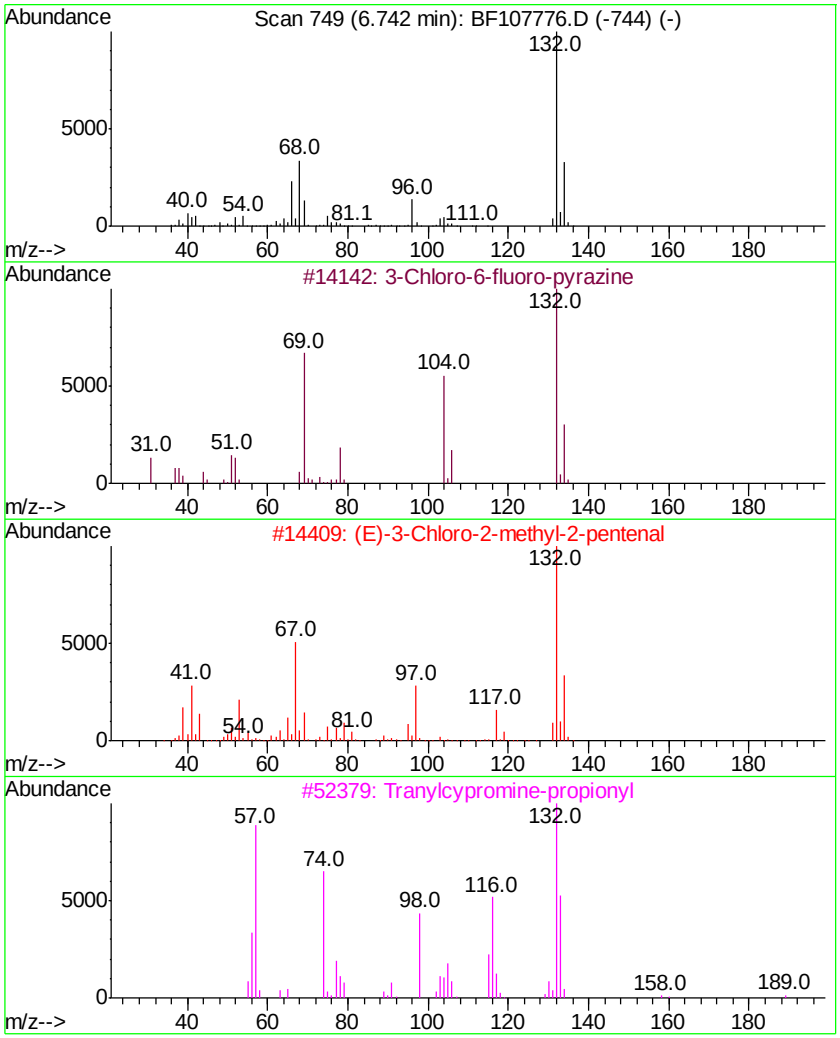
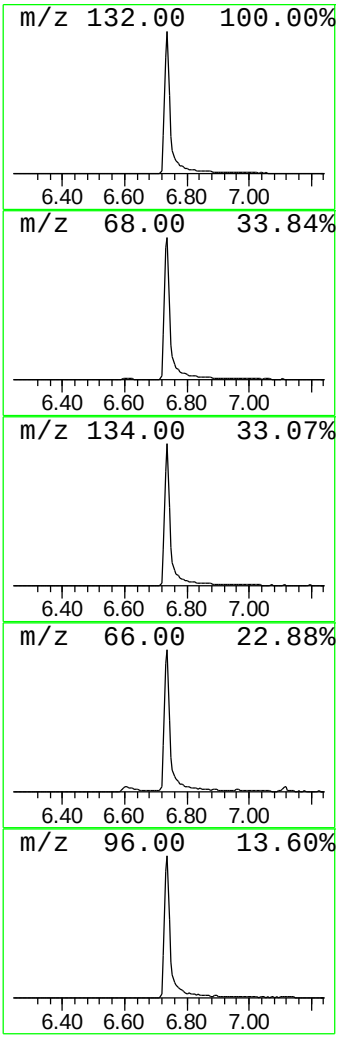
Peak Number 2 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	92.75 ng	3347910	1,4-Dichlorobenzene-d4	6.96

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	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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Acq On : 28 Jul 2018 5:36
Operator : JU/SJ
Sample : J4199-01
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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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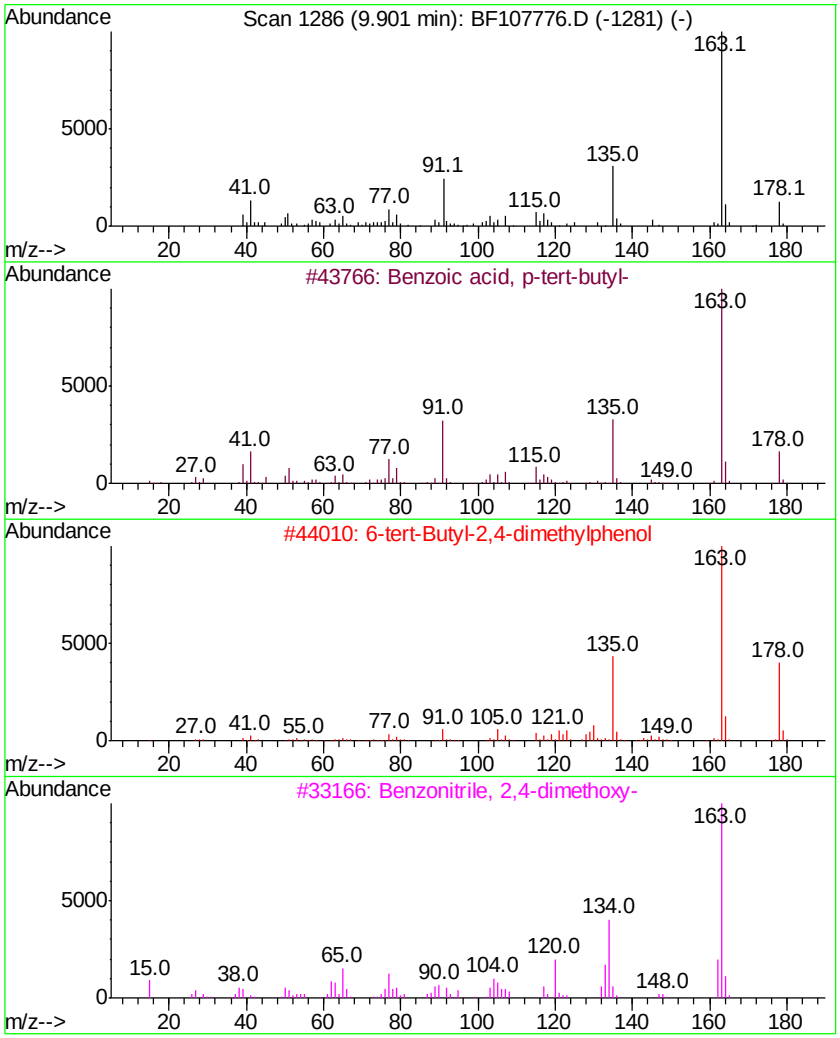
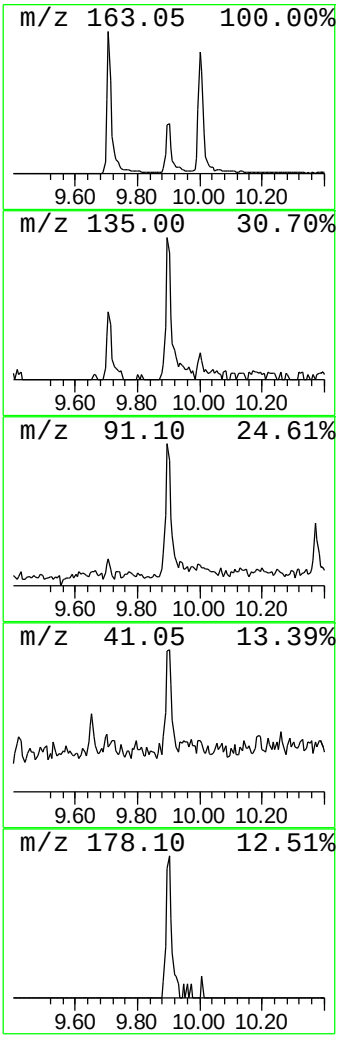
Peak Number 4 Benzoic acid, p-tert-butyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.90	2.07 ng	102677	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	97
2	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	80
3	Benzonitrile, 2,4-dimethoxy-	163	C9H9NO2	004107-65-7	59
4	Silane, (4-ethylphenyl)trimethyl-	178	C11H18Si	017988-50-0	58
5	2-Propenal, 3-(2,6,6-trimethyl-1...	178	C12H18O	004951-40-0	58





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Acq On : 28 Jul 2018 5:36
Operator : JU/SJ
Sample : J4199-01
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MW-33

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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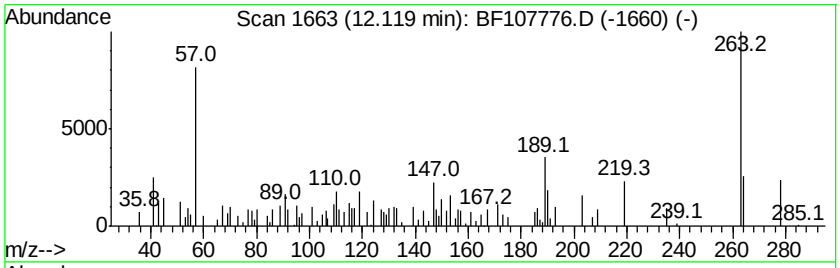
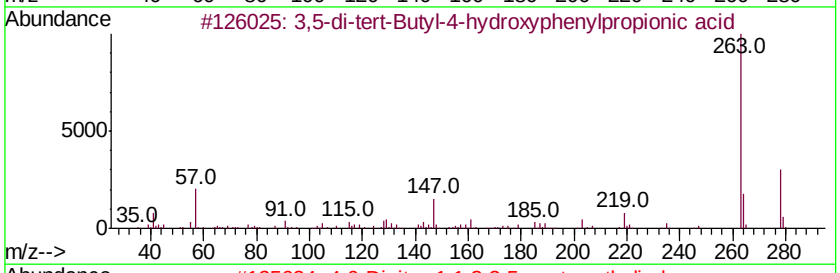
****

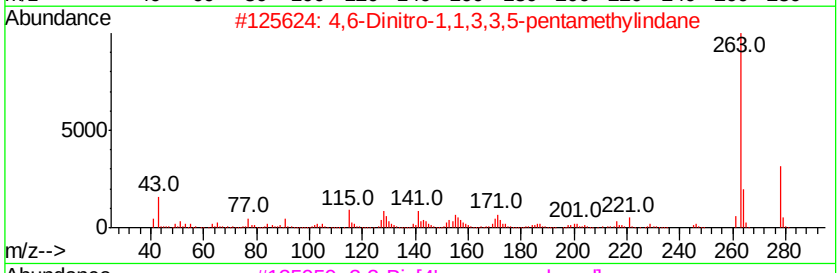
Peak Number 5 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 6

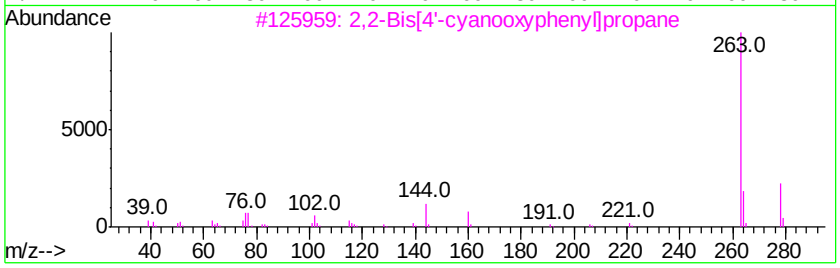
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.12	2.21 ng	118270	Phenanthrene-d10	11.50

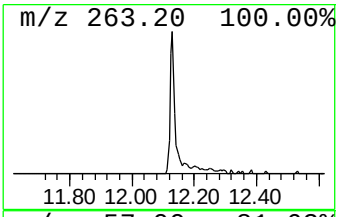
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-di-tert-Butyl-4-hydroxyphenyl...	278	C17H26O3	020170-32-5	94
2	4,6-Dinitro-1,1,3,3,5-pentamethyl...	278	C14H18N2O4	000116-66-5	53
3	2,2-Bis[4'-cyanooxyphenyl]propane	278	C17H14N2O2	1000322-13-3	52
4	Trimethyl(2,6 ditert.-butylpheno...	278	C17H30OSi	010416-73-6	50
5	Thiocyanic acid, (1E)-1-[(phenyl...	263	C14H17NS2	1000362-16-2	50

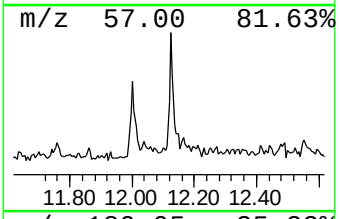


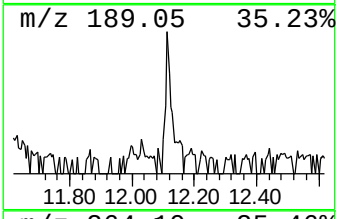


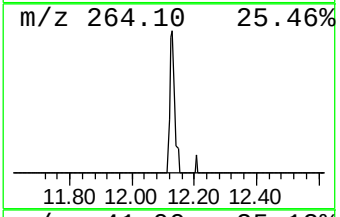


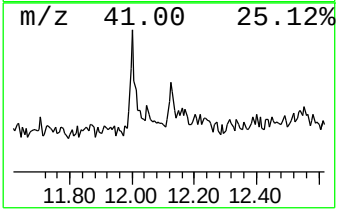












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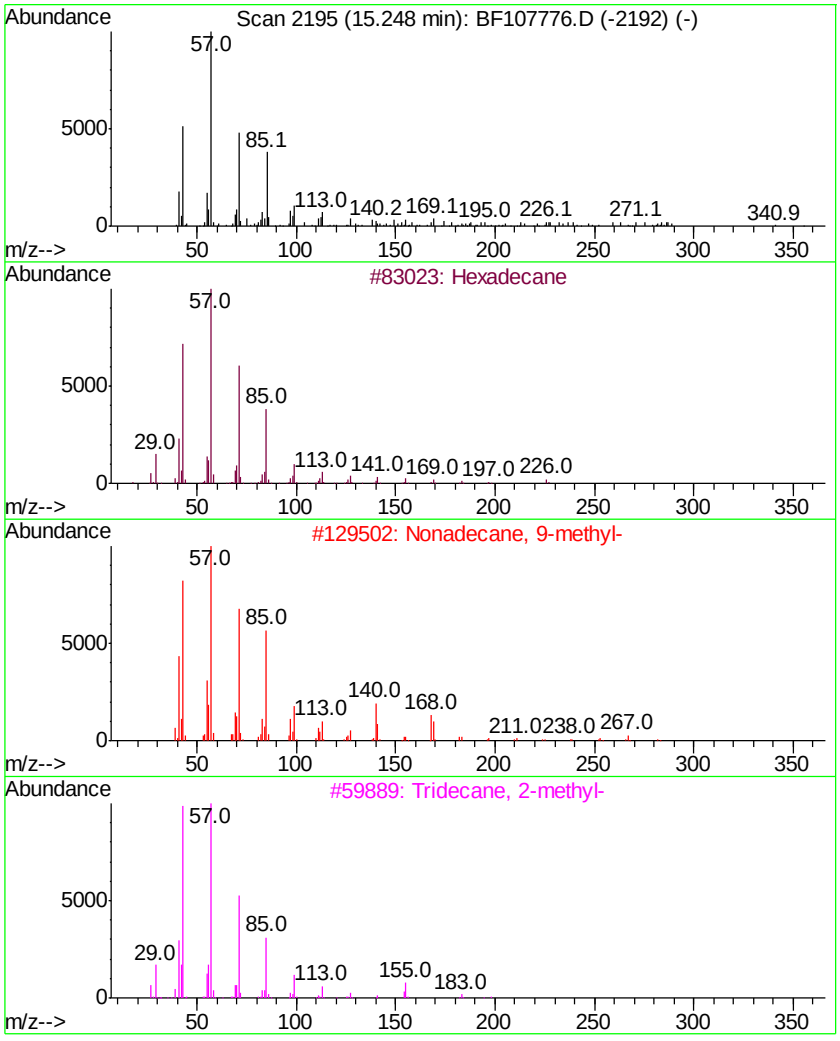
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

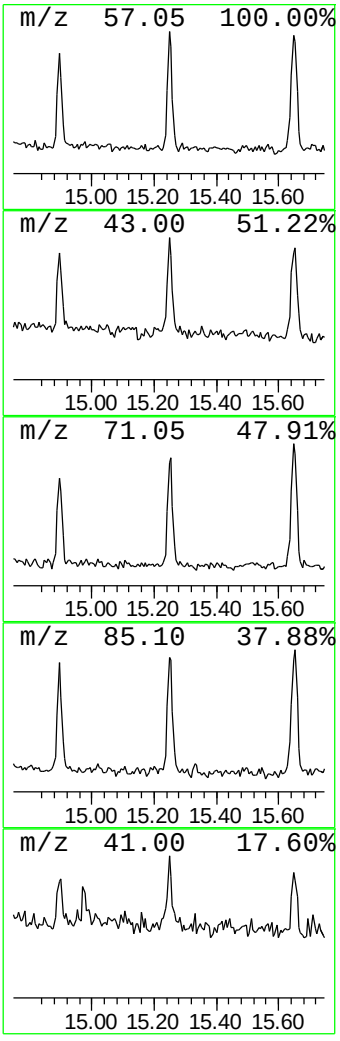
****

Peak Number 6 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	2.39 ng	102020	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	83
3	Tridecane, 2-methyl-	198	C14H30	001560-96-9	80
4	Heptadecane	240	C17H36	000629-78-7	80
5	Pentadecane	212	C15H32	000629-62-9	80





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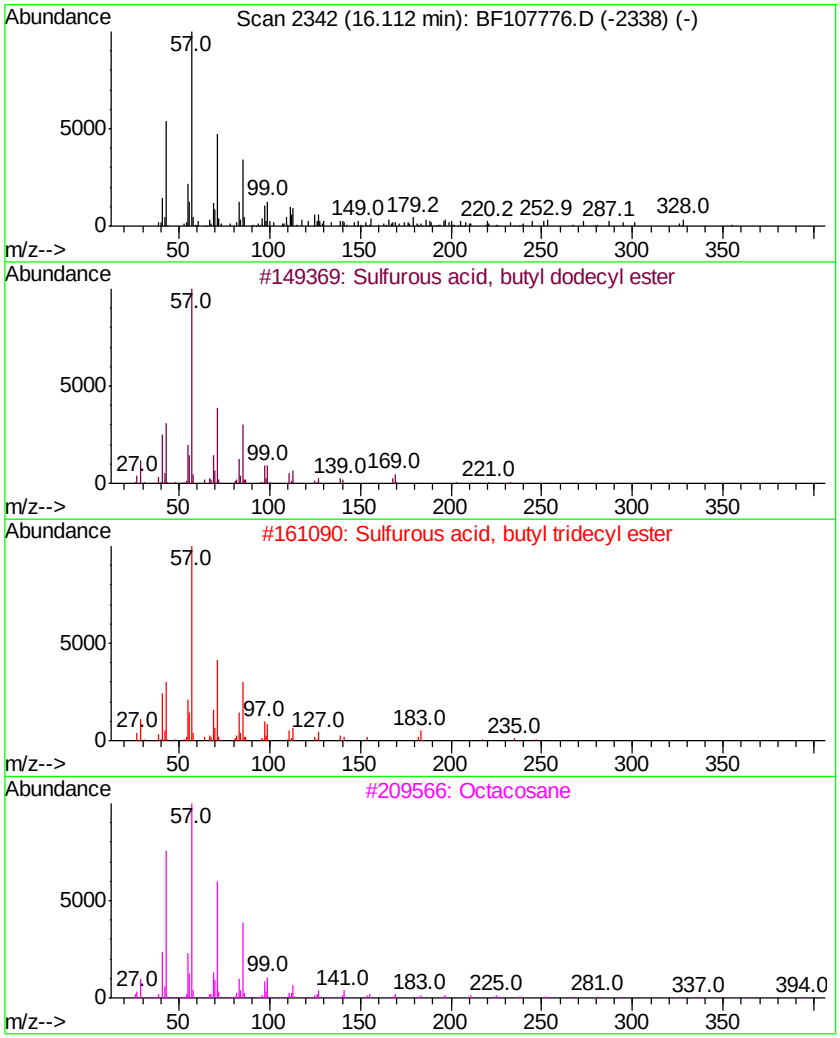
TIC Integration Parameters: LSCINT.P

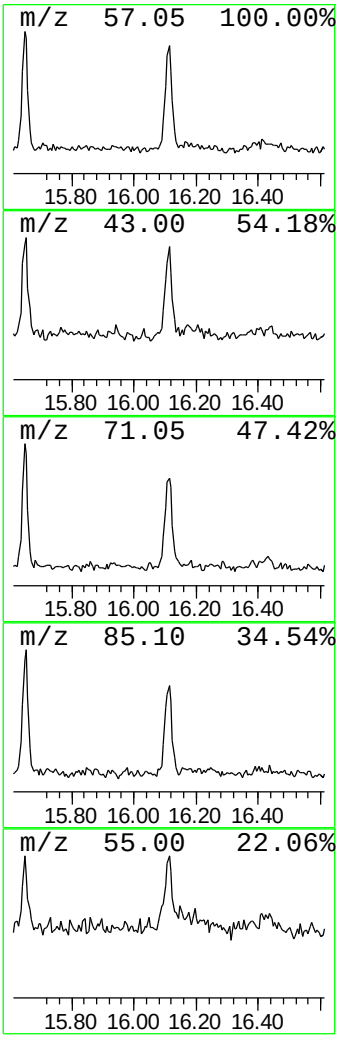
****

Peak Number 7 Sulfurous acid, butyl dodec... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	2.73 ng	116564	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	80
2	Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
3	Octacosane	394	C28H58	000630-02-4	74
4	Hexatriacontane	507	C36H74	000630-06-8	72
5	Tetratetracontane	619	C44H90	007098-22-8	68





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	5.4	ng	196314	1	6.96	721891	20.0
unknown6.74	6.74	92.8	ng	3347910	1	6.96	721891	20.0
Benzoic acid, p-t...	9.90	2.1	ng	102677	3	10.00	990003	20.0
3,5-di-tert-Butyl...	12.12	2.2	ng	118270	4	11.50	1071790	20.0
Hexadecane	15.25	2.4	ng	102020	6	15.68	854225	20.0
Sulfurous acid, b...	16.11	2.7	ng	116564	6	15.68	854225	20.0