LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099634.D
Acq On : 18 Oct 2017 23:05
Operator : SJ/JU
Sample : I5931-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BR-01-101617

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	5.040	499	502	512	rBV	86809	104446	10.92%	0.995%
2	5.451	569	572	591	rBV	709900	714547	74.68%	6.807%
3	6.469	741	745	764	rBV	858036	829761	86.72%	7.904%
4	6.598	764	767	778	rVB	992445	820235	85.72%	7.813%
5	6.828	802	806	813	rBV	640333	517232	54.06%	4.927%
6	6.981	829	832	839	rBV	706195	572514	59.83%	5.454%
7	7.392	898	902	911	rBV	519245	452088	47.25%	4.306%
8	8.110	1020	1024	1027	rBV	697108	595904	62.28%	5.676%
9	9.180	1202	1206	1209	rBV	1192614	956836	100.00%	9.115%
10	9.575	1269	1273	1275	rBV	18613	15185	1.59%	0.145%
11	9.863	1318	1322	1328	rVB	591011	507429	53.03%	4.834%
12	10.651	1453	1456	1465	rBV	508748	419826	43.88%	3.999%
13	10.751	1470	1473	1479	rBV2	12255	13518	1.41%	0.129%
14	11.351	1571	1575	1578	rBV	517520	456010	47.66%	4.344%
15	11.727	1636	1639	1642	rBV	242366	173558	18.14%	1.653%
16	11.863	1659	1662	1671	rBV2	21349	27964	2.92%	0.266%
17	12.410	1752	1755	1757	rBV	420991	387689	40.52%	3.693%
18	12.433	1757	1759	1762	rVB	678895	500884	52.35%	4.771%
19	12.516	1770	1773	1777	rBV	156992	126422	13.21%	1.204%
20	12.751	1809	1813	1817	rVB5	11673	14831	1.55%	0.141%
21	12.927	1839	1843	1846	rVB	1054735	861677	90.05%	8.208%
22	13.116	1870	1875	1878	rBV4	19366	28521	2.98%	0.272%
23	13.239	1893	1896	1898	rBV	17306	14482	1.51%	0.138%
24	13.674	1966	1970	1973	rBV3	32257	38331	4.01%	0.365%
25	13.815	1991	1994	2000	rBV2	35968	44645	4.67%	0.425%
26	13.910	2007	2010	2013	rBV2	21021	20638	2.16%	0.197%
27	13.992	2020	2024	2031	rBV	648261	584881	61.13%	5.571%
28	14.133	2044	2048	2051	rBV4	13349	18077	1.89%	0.172%
29	14.433	2096	2099	2101	rBV	33423	31526	3.29%	0.300%
30	14.739	2147	2151	2154	rBV2	34273	44901	4.69%	0.428%
31	15.068	2203	2207	2211	rBV	40119	49209	5.14%	0.469%
32	15.457	2267	2273	2280	rBV	407672	509541	53.25%	4.854%
33	15.862	2339	2342	2346	rVB	36775	44551	4.66%	0.424%

LSC Area Percent Report

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Instrument : BNA_F
ClientSampleId : BR-01-101617

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

Sum of corrected areas: 10497859

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101817\
Data File : BF099634.D
Acq On : 18 Oct 2017 23:05
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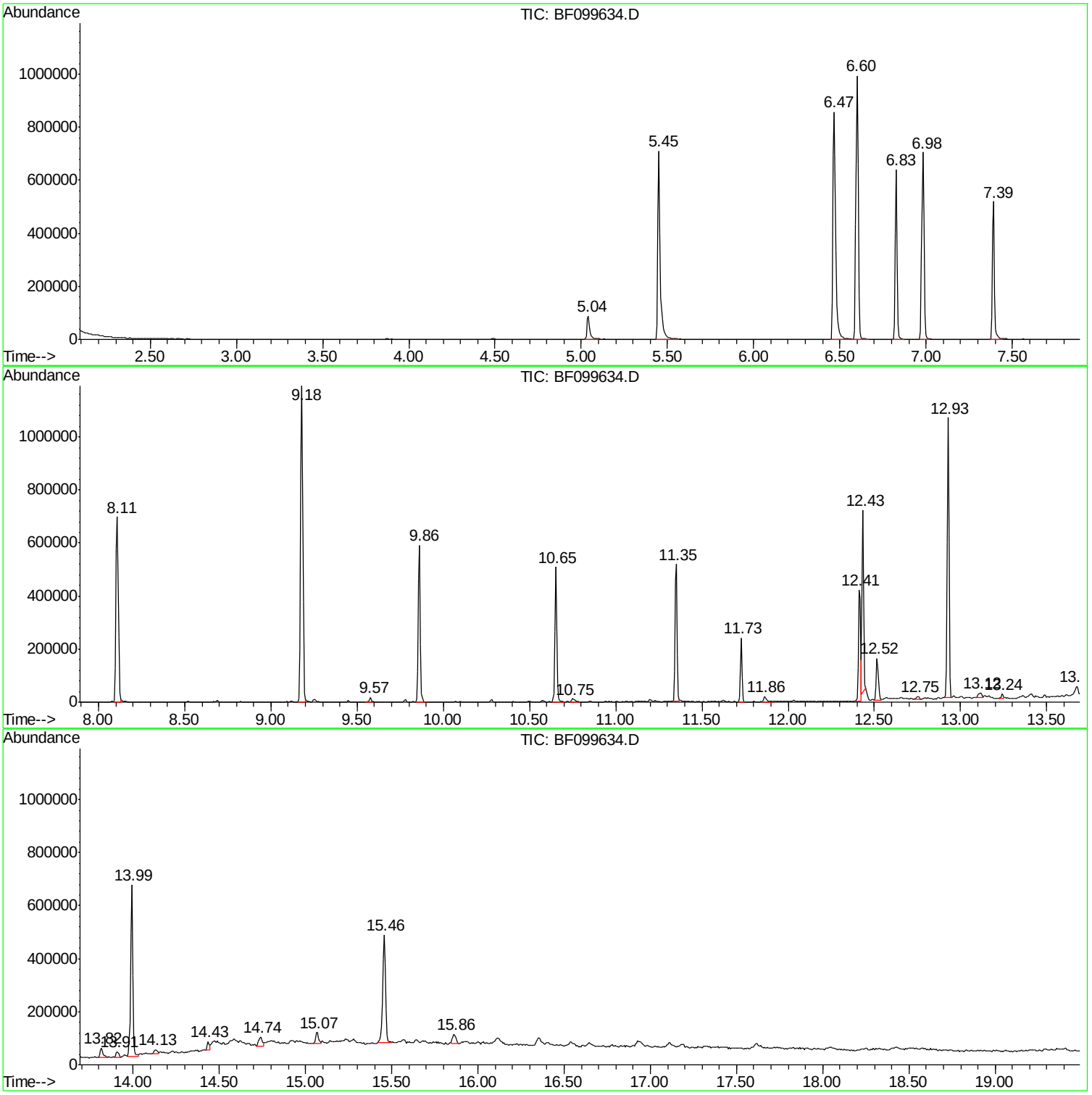
Sample : I5931-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BR-01-101617

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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Sample : I5931-01 2X
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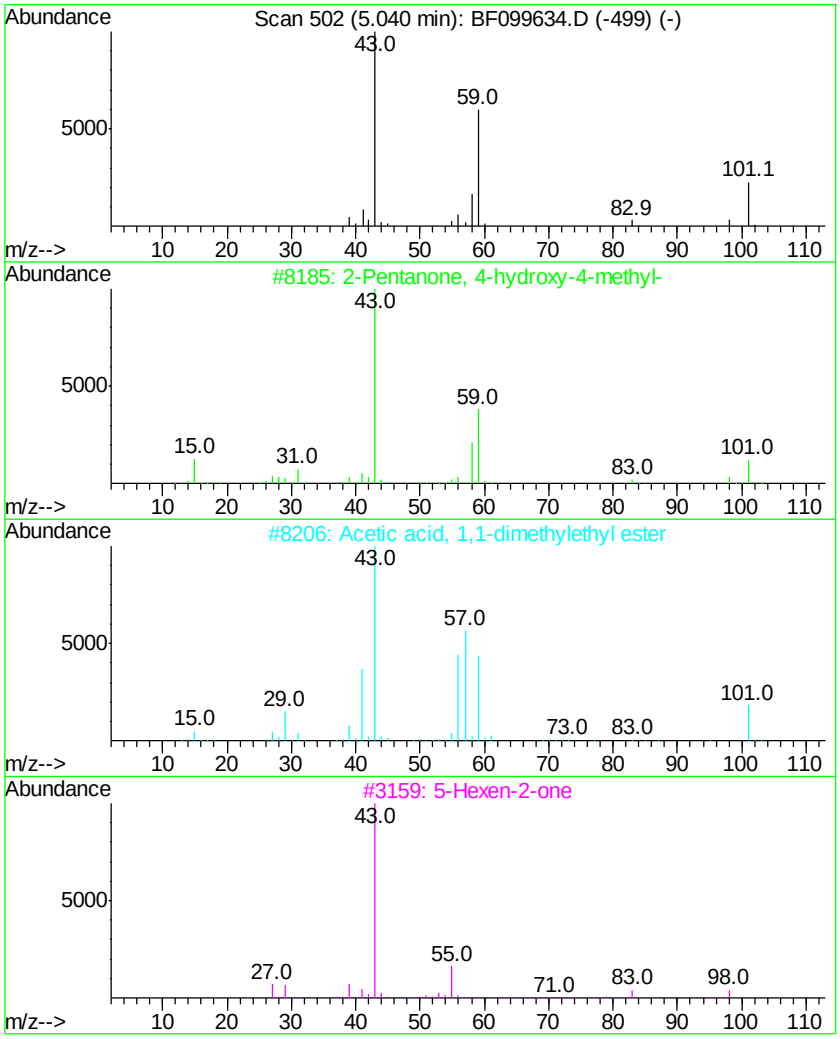
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

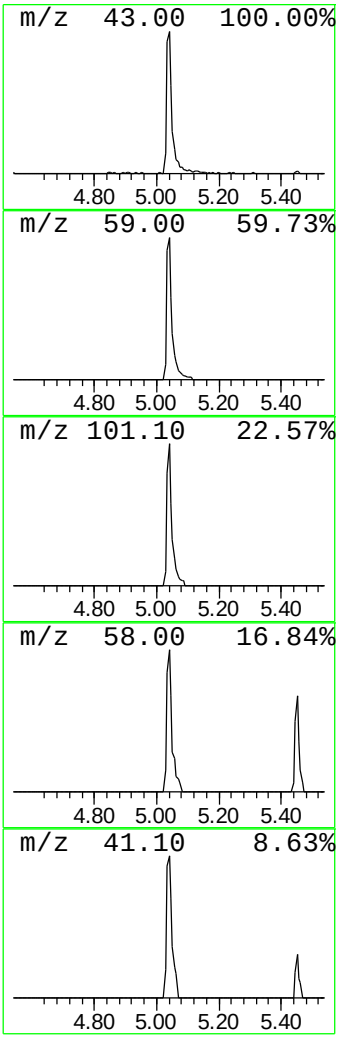
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	4.04 ng	104446	1,4-Dichlorobenzene-d4	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Acetone	58	C3H6O	000067-64-1	9
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9





Library Search Compound Report

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Data File : BF099634.D
Acq On : 18 Oct 2017 23:05
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Sample : I5931-01 2X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BR-01-101617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

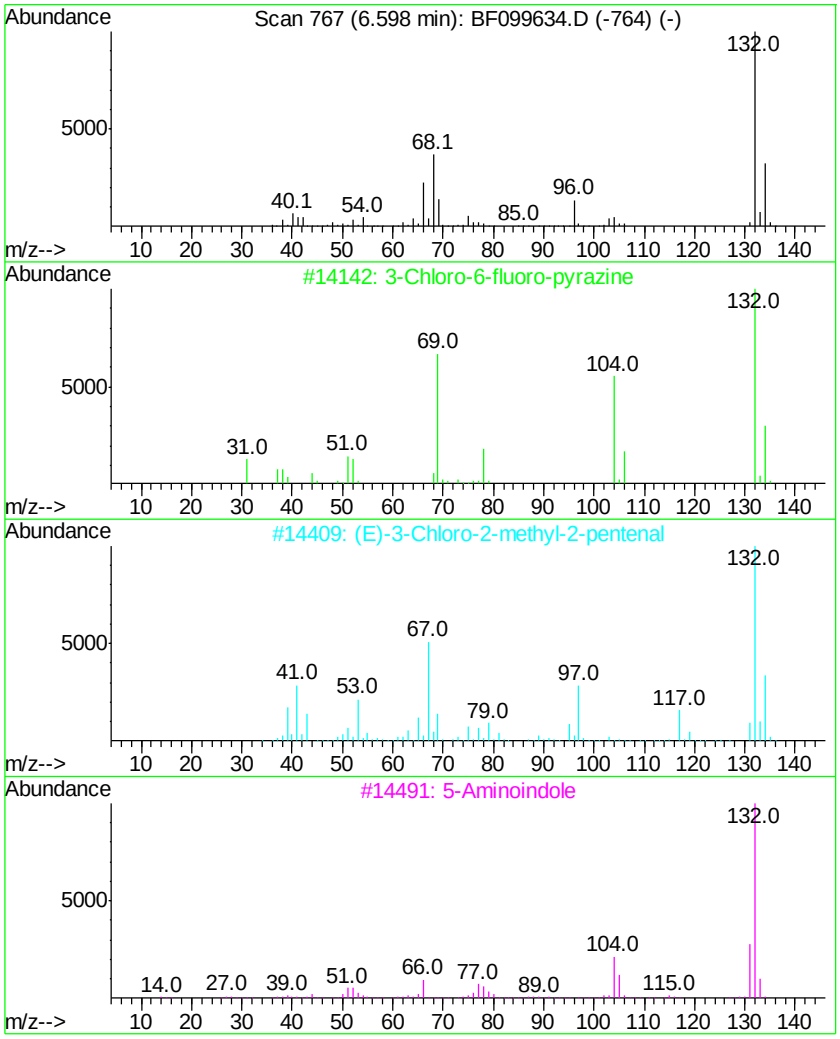
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

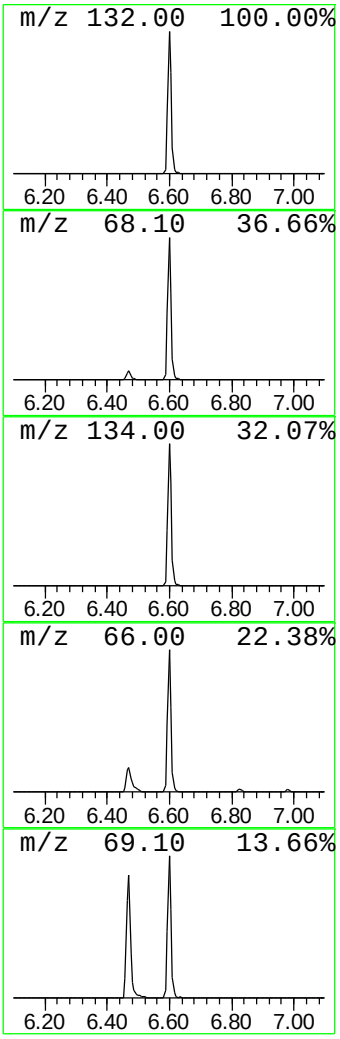
****

Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	31.72 ng	820235	1,4-Dichlorobenzene-d4	6.83

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : I5931-01 2X
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Instrument : BNA_F
ClientSampleId : BR-01-101617

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

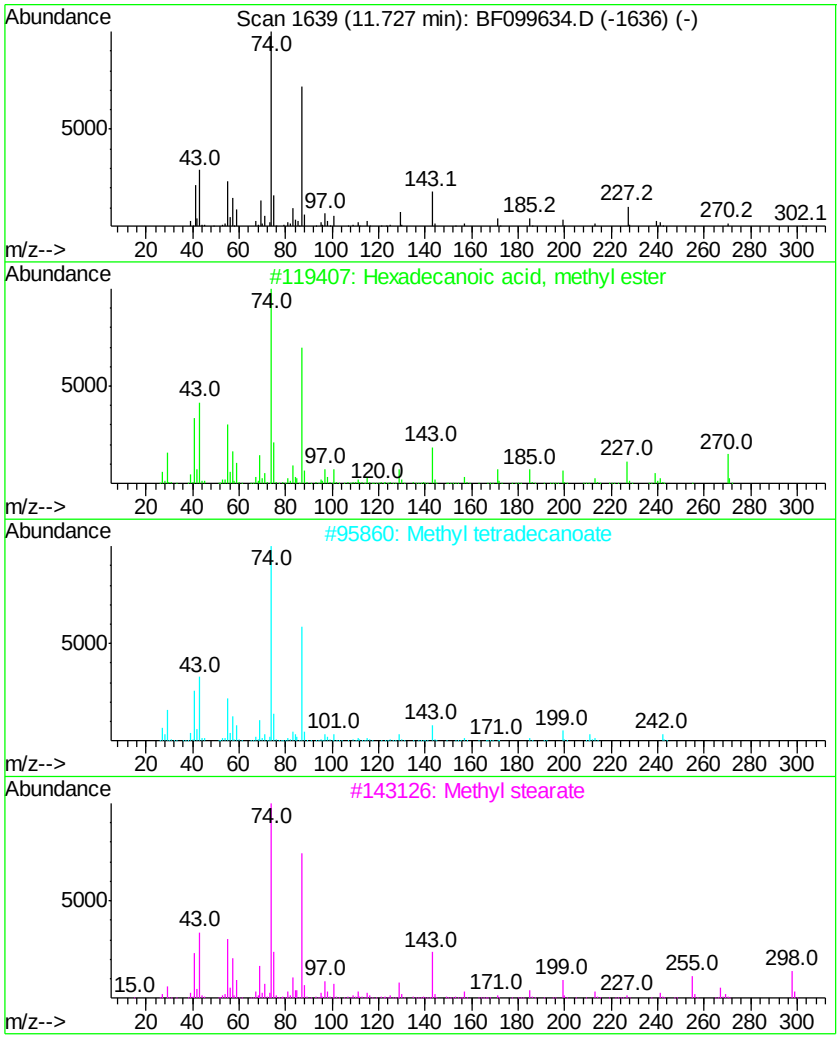
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

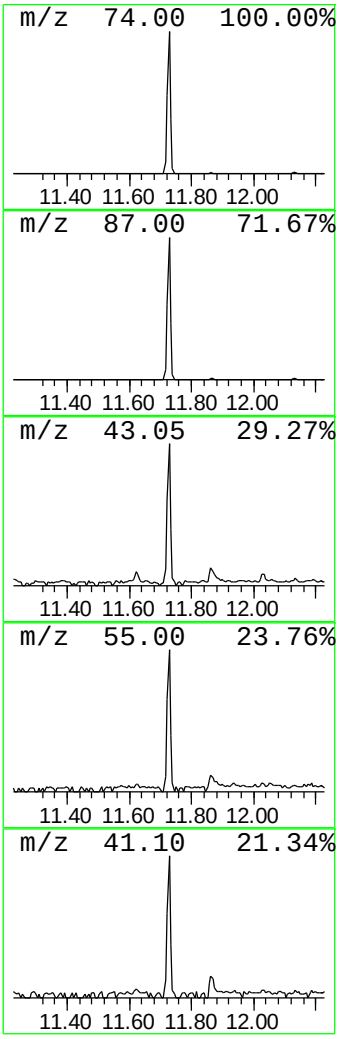
****

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	7.61 ng	173558	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
3	Methyl stearate	298	C19H38O2	000112-61-8	87
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	86





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TIC Library : C:\DATABASE\NIST11.L
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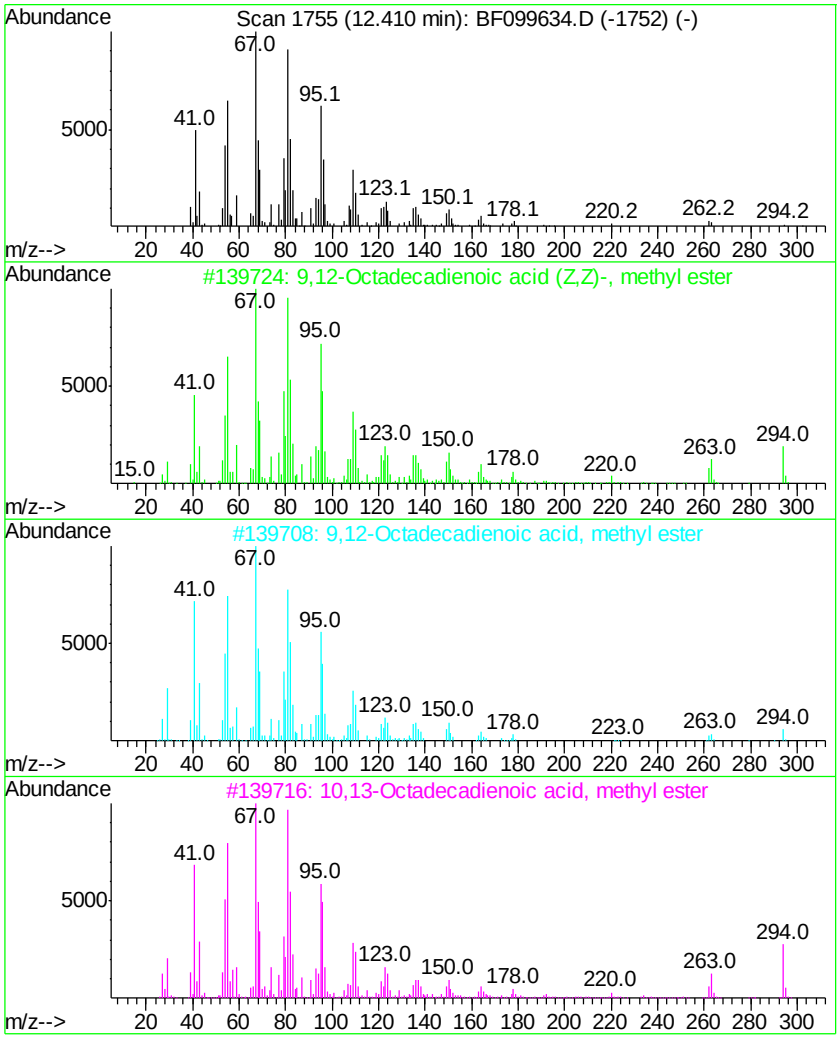
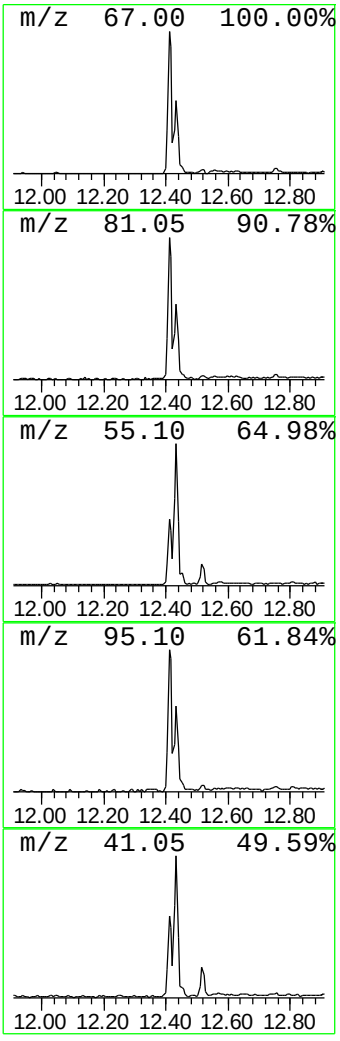
****
Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.41	17.00 ng	387689	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
4	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	99
5	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99





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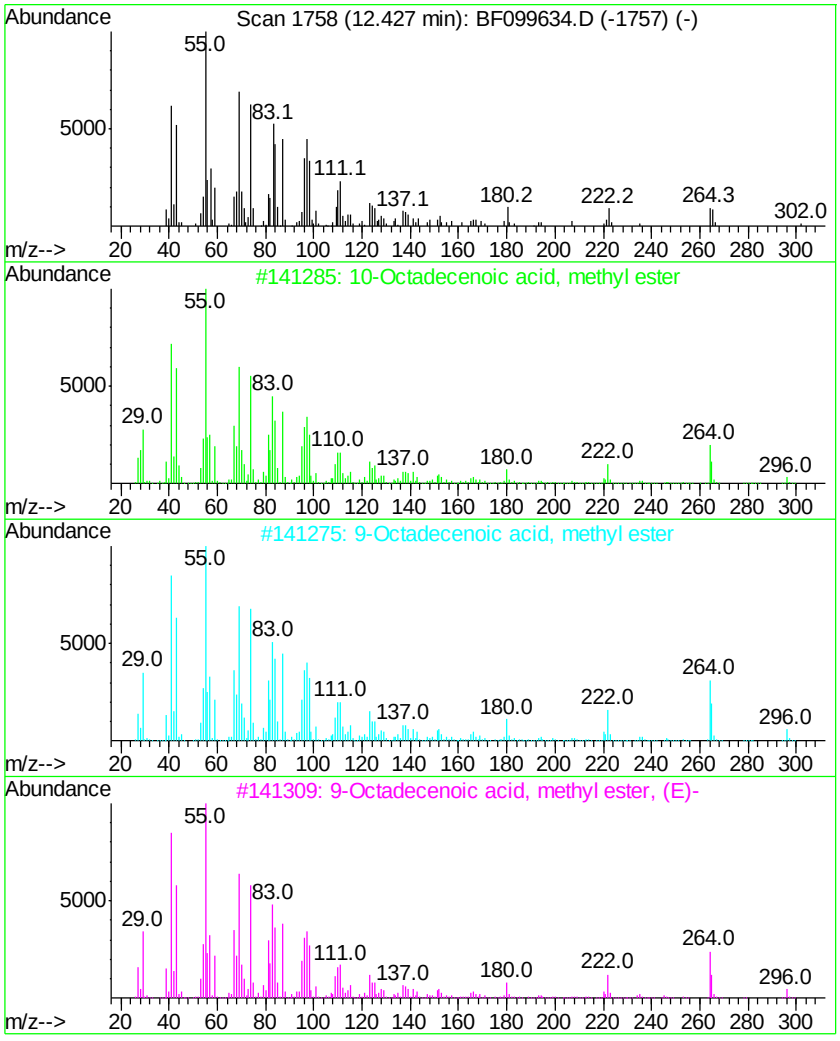
TIC Integration Parameters: LSCINT.P

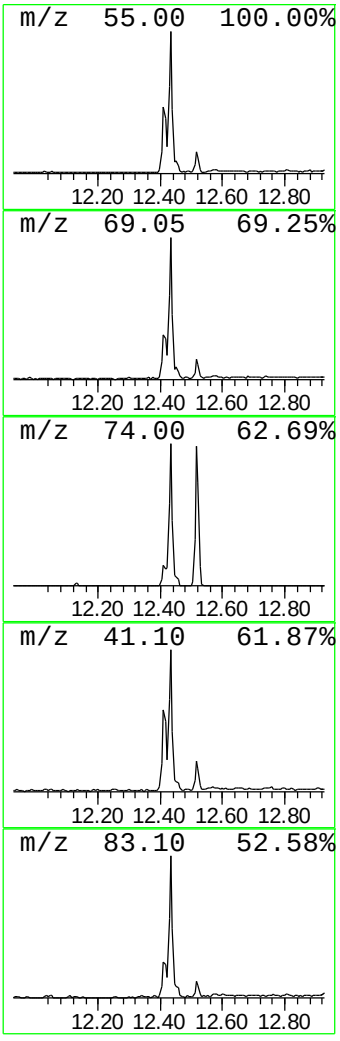
****

Peak Number 6 10-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	21.97 ng	500884	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
3	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
4	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	99
5	8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	98





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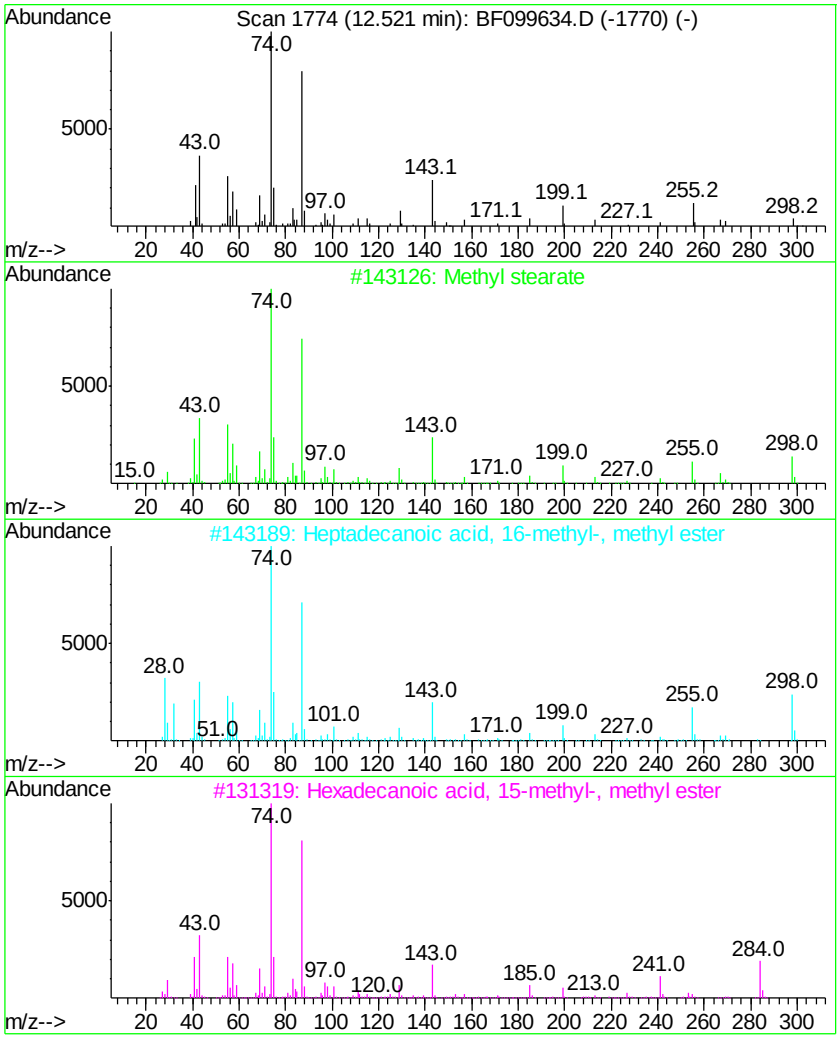
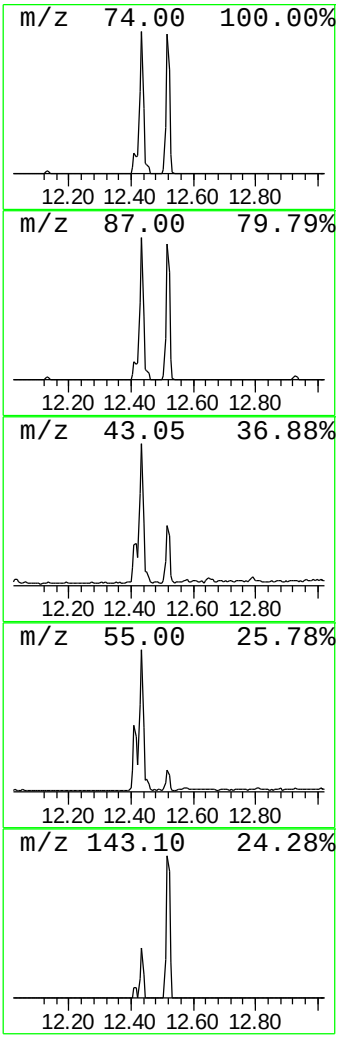
Peak Number 7 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	5.54 ng	126422	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	96
3	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
4	Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	91
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	90





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...	5.04	4.0	ng	104446	1	6.83	517232	20.0
unknown6.60	6.60	31.7	ng	820235	1	6.83	517232	20.0
Hexadecanoic acid...	11.73	7.6	ng	173558	4	11.35	456010	20.0
9,12-Octadecadien...	12.41	17.0	ng	387689	4	11.35	456010	20.0
10-Octadecenoic a...	12.43	22.0	ng	500884	4	11.35	456010	20.0
Methyl stearate	12.52	5.5	ng	126422	4	11.35	456010	20.0