LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF041219\
Data File : BF113758.D
Acq On : 13 Apr 2019 00:50
Operator : JU/SJ
Sample : K2204-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-041119

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-BF040319.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	5.298	544	546	574	rBV	151979	378396	6.02%	1.323%
2	6.340	720	723	739	rBV	159054	397273	6.32%	1.389%
3	6.451	739	742	762	rVB	332885	485819	7.73%	1.699%
4	6.669	776	779	799	rVB	546426	600311	9.55%	2.099%
5	6.828	803	806	819	rBV	347045	352946	5.61%	1.234%
6	7.245	874	877	891	rBV	121725	235024	3.74%	0.822%
7	7.957	994	998	1018	rBV	636122	749436	11.92%	2.620%
8	9.028	1177	1180	1191	rBV	497105	482719	7.68%	1.688%
9	9.704	1291	1295	1299	rBV	777948	720294	11.46%	2.518%
10	10.498	1427	1430	1442	rVB	203704	251253	4.00%	0.878%
11	10.716	1461	1467	1470	rBV	78197	71426	1.14%	0.250%
12	11.186	1544	1547	1549	rBV	831862	736413	11.71%	2.575%
13	11.210	1549	1551	1558	rVV	285216	270305	4.30%	0.945%
14	11.504	1599	1601	1605	rVB2	117837	94577	1.50%	0.331%
15	11.580	1610	1614	1618	rBV	2885761	2572476	40.92%	8.994%
16	11.722	1635	1638	1644	rBV2	127988	166716	2.65%	0.583%
17	11.798	1648	1651	1654	rBV	70312	71383	1.14%	0.250%
18	11.898	1661	1668	1671	rBV5	51686	80644	1.28%	0.282%
19	11.980	1679	1682	1687	rBV	76093	70995	1.13%	0.248%
20	12.275	1727	1732	1733	rVV	5075826	6286498	100.00%	21.980%
21	12.292	1733	1735	1741	rVV	5369147	5920218	94.17%	20.700%
22	12.333	1741	1742	1745	rVV	140776	114485	1.82%	0.400%
23	12.369	1745	1748	1751	rVV	1590051	1442355	22.94%	5.043%
24	12.398	1751	1753	1756	rVV	435623	439523	6.99%	1.537%
25	12.427	1756	1758	1768	rVB5	125694	254638	4.05%	0.890%
26	12.627	1789	1792	1800	rVB	415230	446932	7.11%	1.563%
27	12.763	1811	1815	1819	rBV	644644	594814	9.46%	2.080%
28	12.851	1826	1830	1836	rBV3	69486	120376	1.91%	0.421%
29	12.957	1841	1848	1853	rBV3	156106	278309	4.43%	0.973%
30	13.016	1853	1858	1862	rVB4	127805	200200	3.18%	0.700%
31	13.092	1868	1871	1874	rVB	137128	117381	1.87%	0.410%
32	13.198	1884	1889	1895	rBV4	114995	187492	2.98%	0.656%
33	13.522	1939	1944	1948	rVB3	95713	143475	2.28%	0.502%
34	13.757	1981	1984	1987	rBV	141252	125259	1.99%	0.438%

LSC Area Percent Report

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Sample : K2204-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-041119

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-BF040319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.821	1990	1995	1998	rBV2	1087114	1191801	18.96%	4.167%
36	13.980	2019	2022	2029	rVB2	106764	118661	1.89%	0.415%
37	14.286	2071	2074	2076	rBV	149641	138553	2.20%	0.484%
38	14.574	2121	2123	2128	rVB	186217	182190	2.90%	0.637%
39	14.839	2165	2168	2170	rBV	141681	167805	2.67%	0.587%
40	14.886	2173	2176	2182	rVB	241892	252616	4.02%	0.883%
41	15.233	2230	2235	2248	rVB	661775	905401	14.40%	3.166%
42	15.621	2298	2301	2306	rVB	144161	183203	2.91%	0.641%

Sum of corrected areas: 28600591

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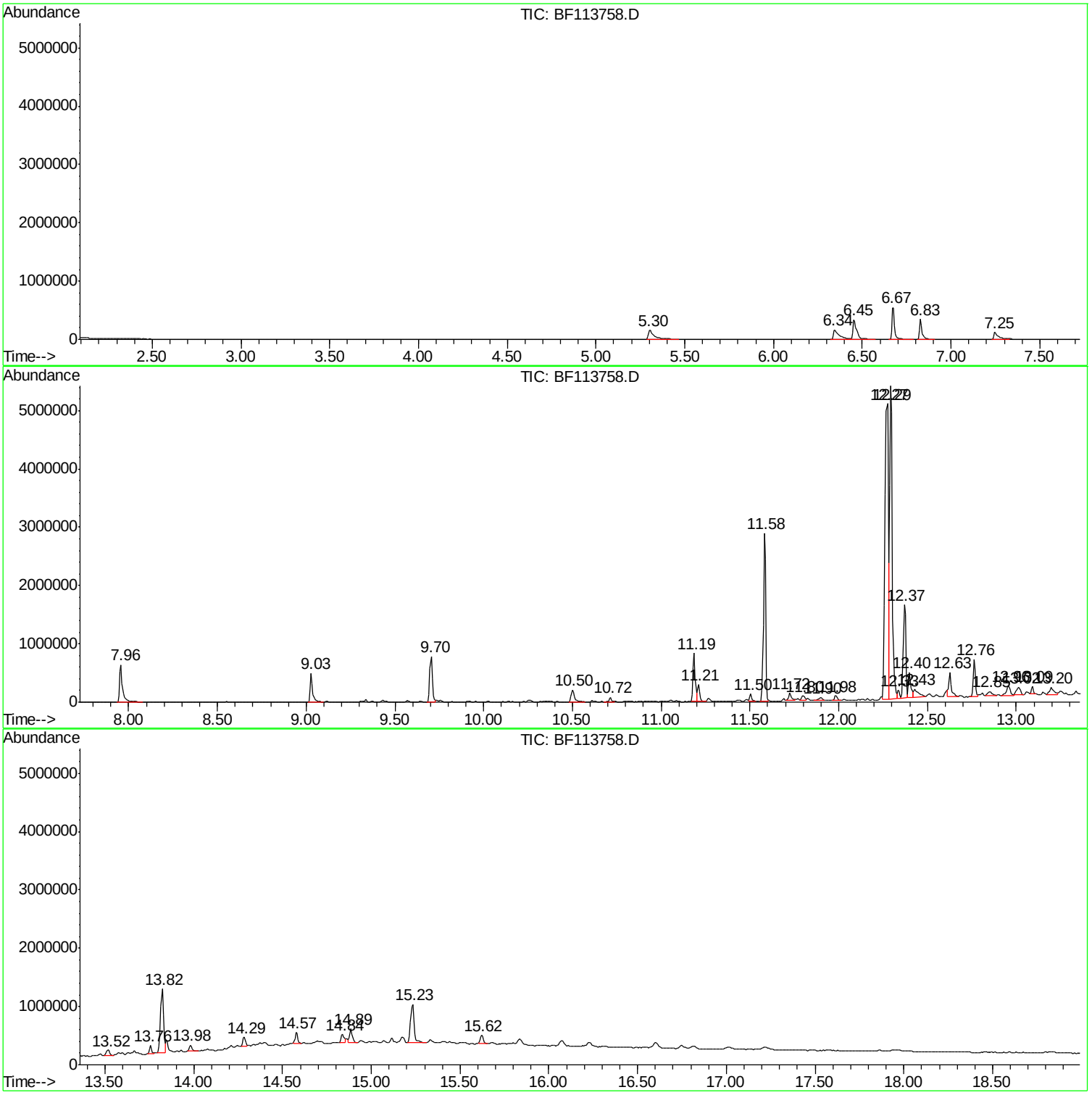
ALS Vial : 23 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TR-04-041119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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Instrument : BNA_F
ClientSampleId : TR-04-041119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
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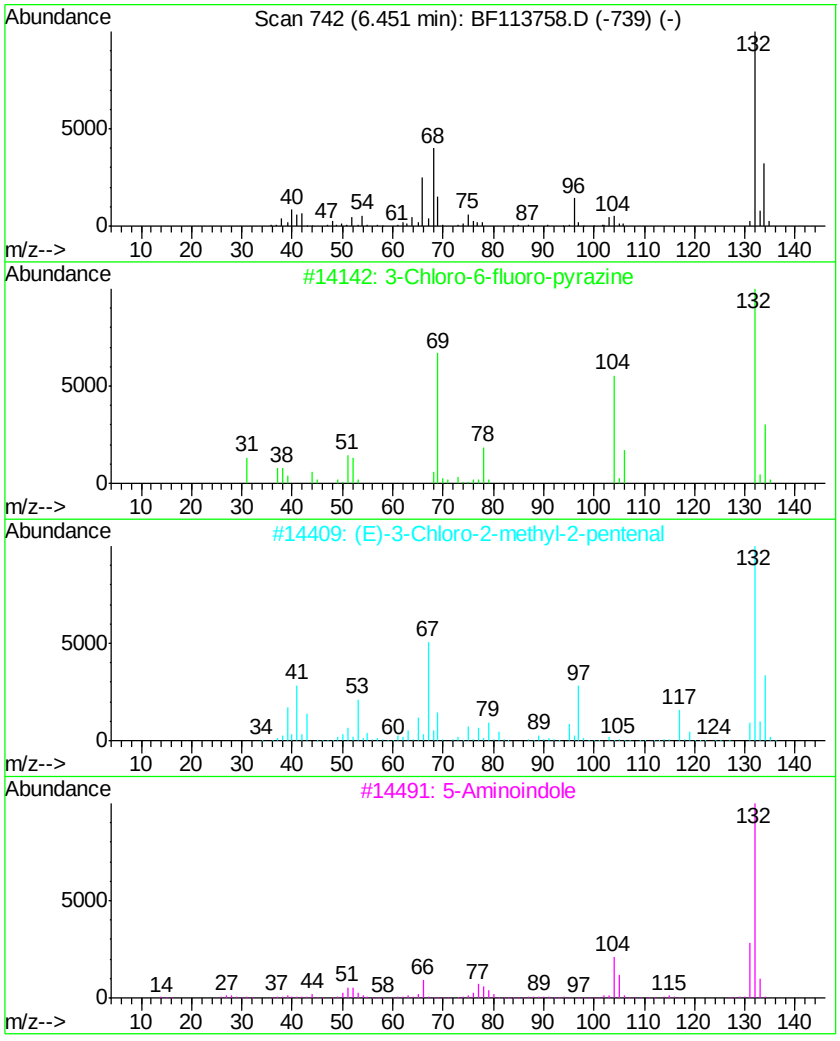
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

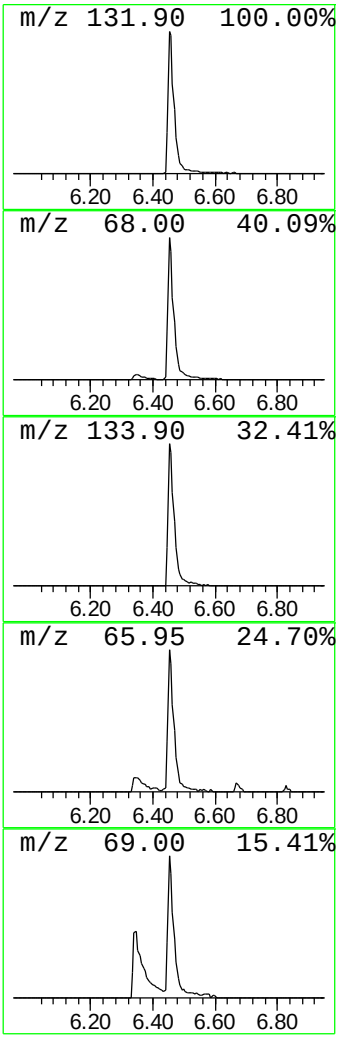
****

Peak Number 1 unknown6.45 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	16.19 ng	485819	1,4-Dichlorobenzene-d4	6.67

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	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1-Isoquinolinemethanol, .alpha.-...	191	C12H17NO	114608-92-3	10





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Sample : K2204-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-041119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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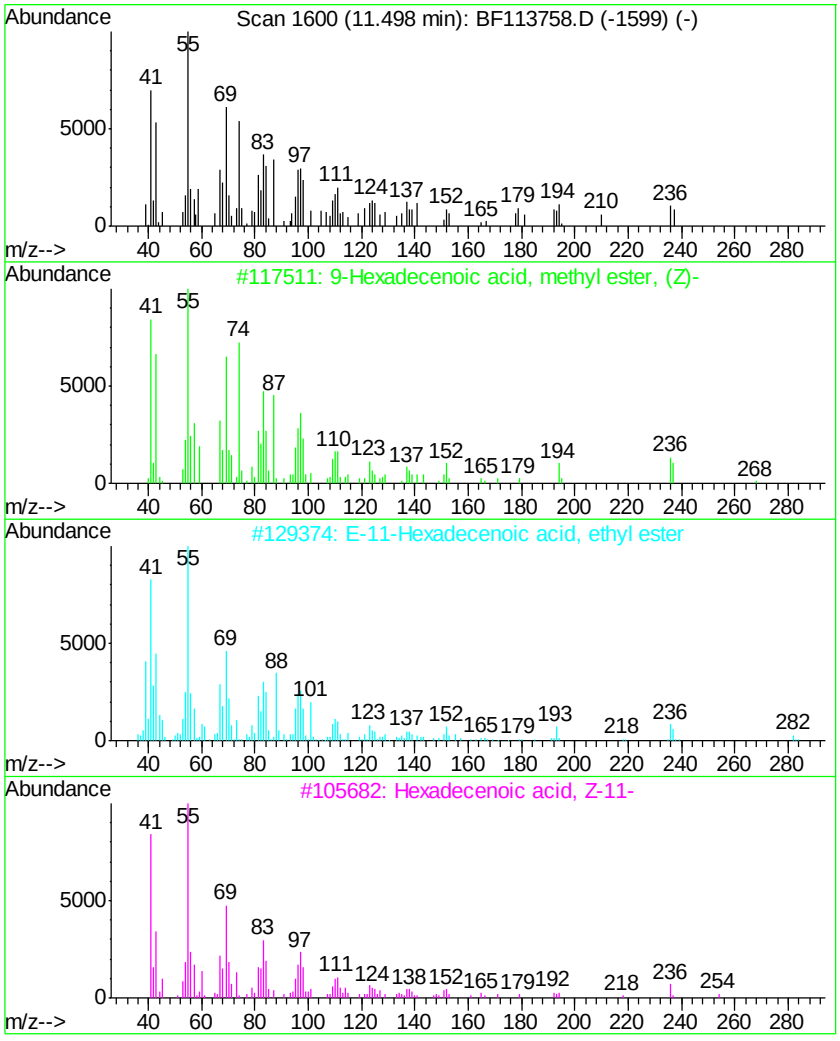
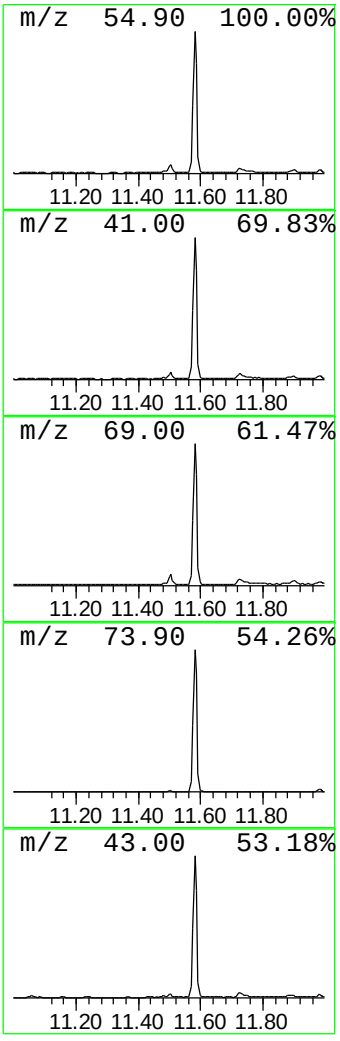
Peak Number 3 9-Hexadecenoic acid, methyl... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.50	2.57 ng	94577	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	90
2	E-11-Hexadecenoic acid, ethyl ester	282	C18H34O2	1000245-71-9	64
3	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	64
4	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	52
5	Chloromethyl 6-chlorododecanoate	282	C13H24Cl2O2	080419-02-9	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF041219\
Data File : BF113758.D
Acq On : 13 Apr 2019 00:50
Operator : JU/SJ
Sample : K2204-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-041119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

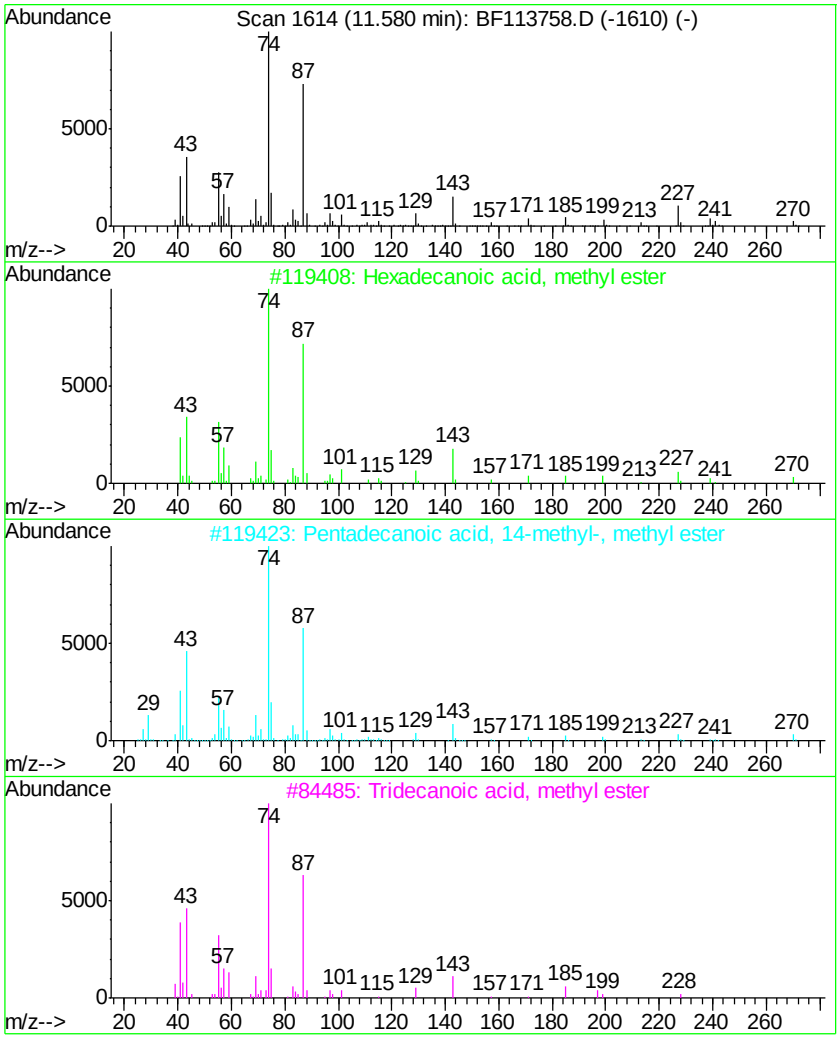
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

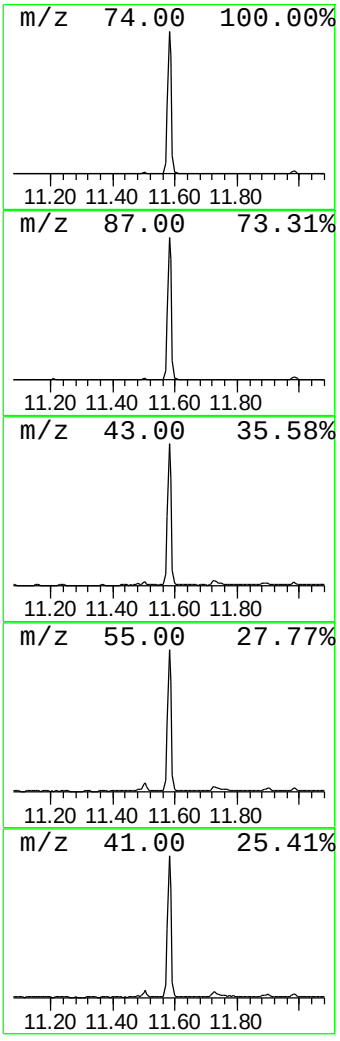
****

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.58	69.87 ng	2572480	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





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Sample : K2204-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-041119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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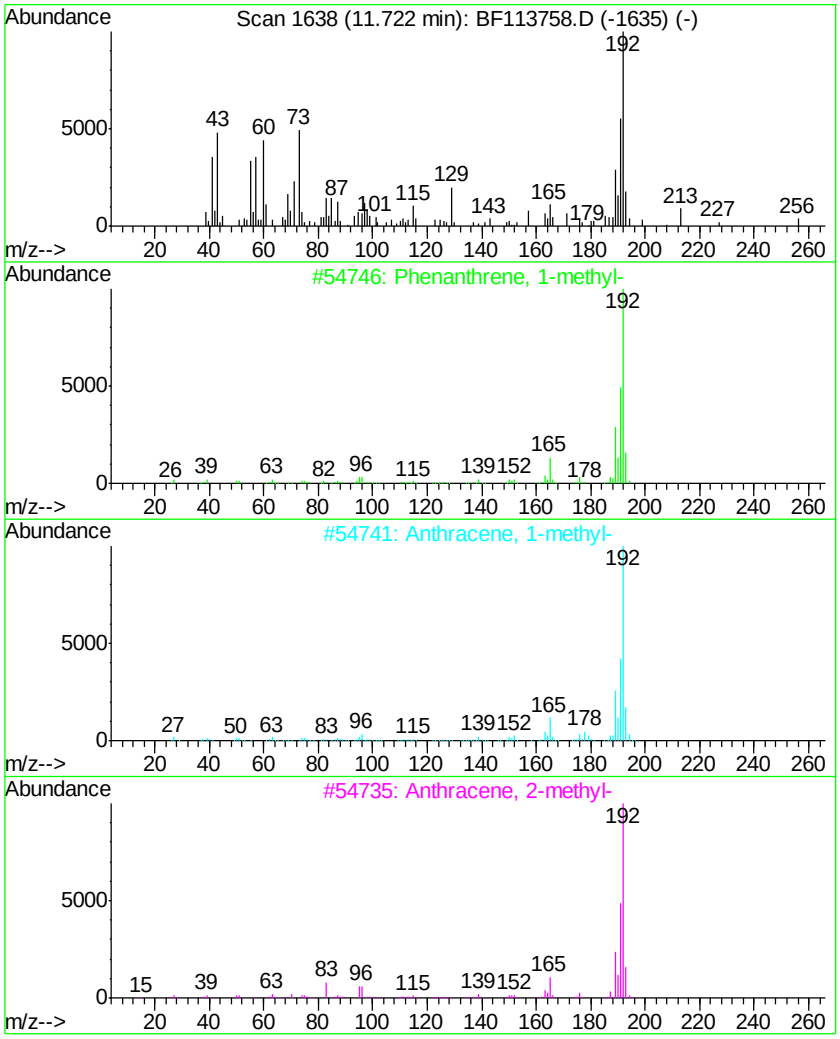
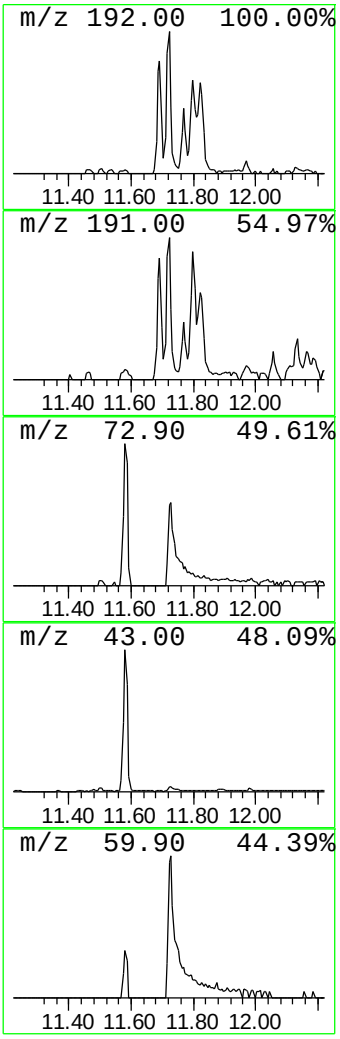
Peak Number 5 Phenanthrene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.72	4.53 ng	166716	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	78
2	Anthracene, 1-methyl-	192	C15H12	000610-48-0	78
3	Anthracene, 2-methyl-	192	C15H12	000613-12-7	78
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	78
5	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	78





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Misc :
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Instrument : BNA_F
ClientSampleId : TR-04-041119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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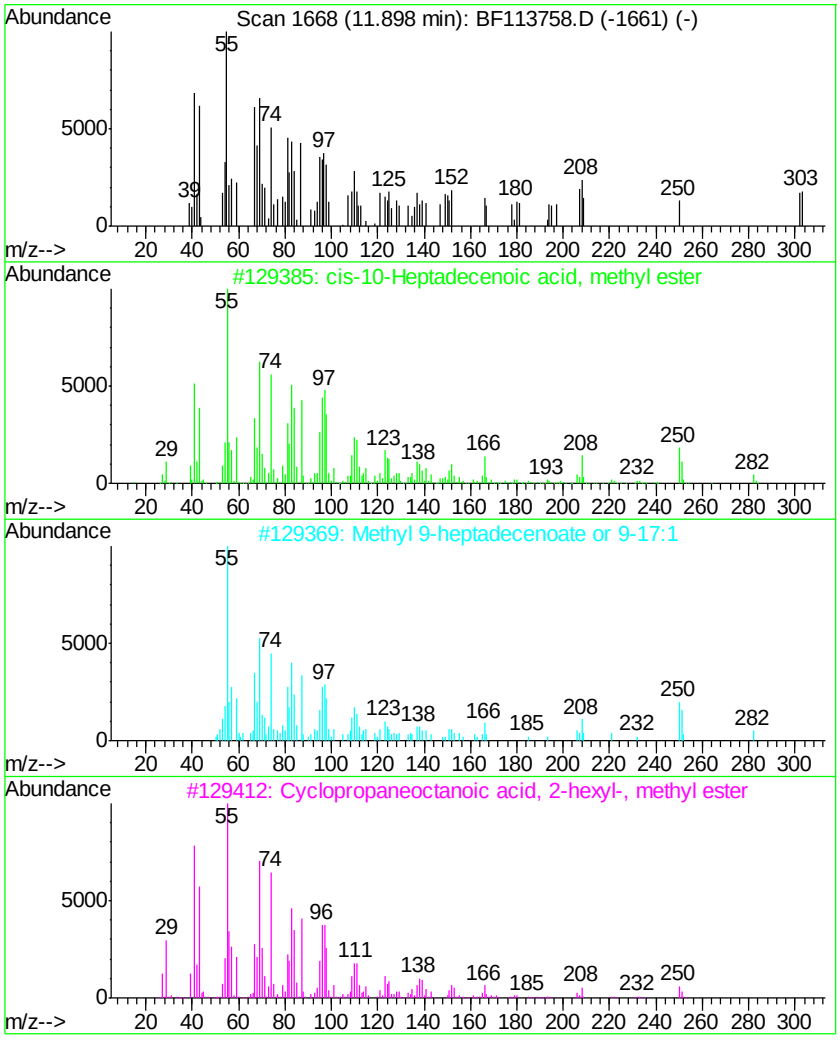
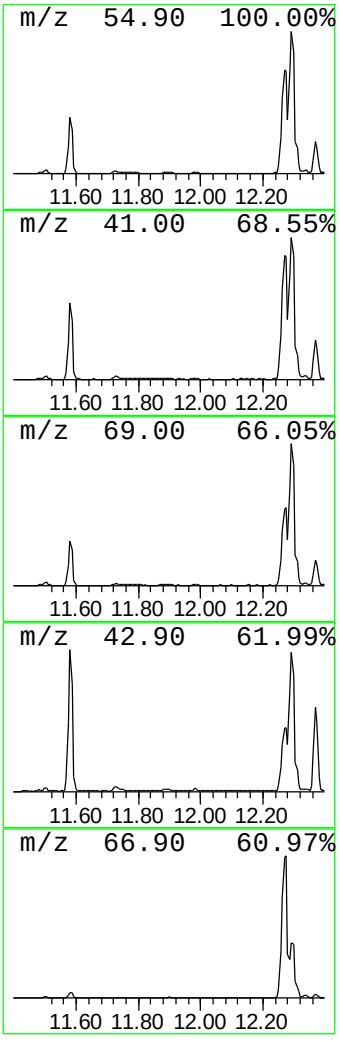
****

Peak Number 6 cis-10-Heptadecenoic acid, ... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	2.19 ng	80644	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	70
2	Methyl 9-heptadecenoate or 9-17:1	282	C18H34O2	1000336-38-0	68
3	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	64
4	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	58
5	9-Oxabicyclo[6.1.0]nonane, cis-	126	C8H14O	004925-71-7	55





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

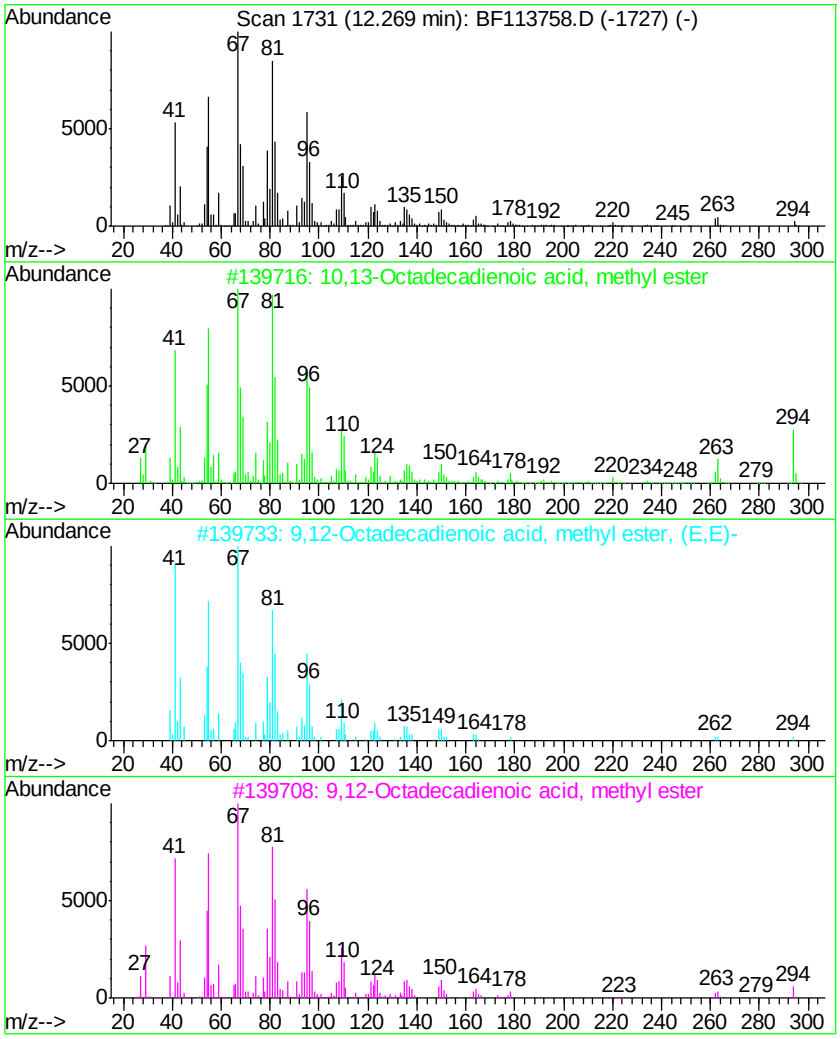
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

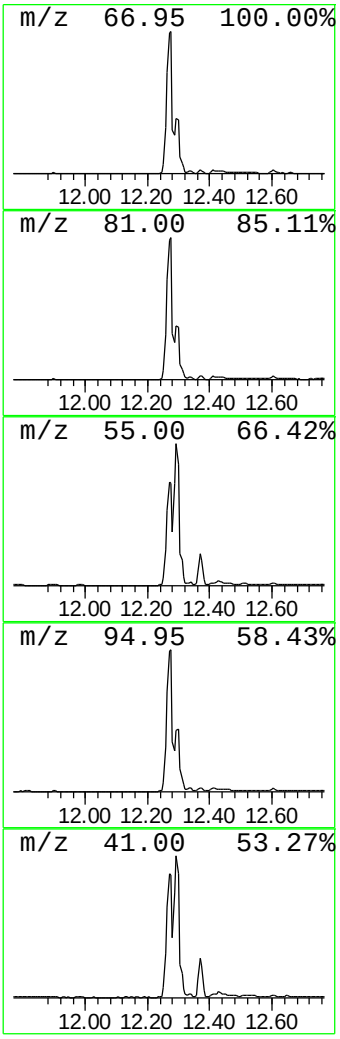
****

Peak Number 7 10,13-Octadecadienoic acid,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	170.73 ng	6286500	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99





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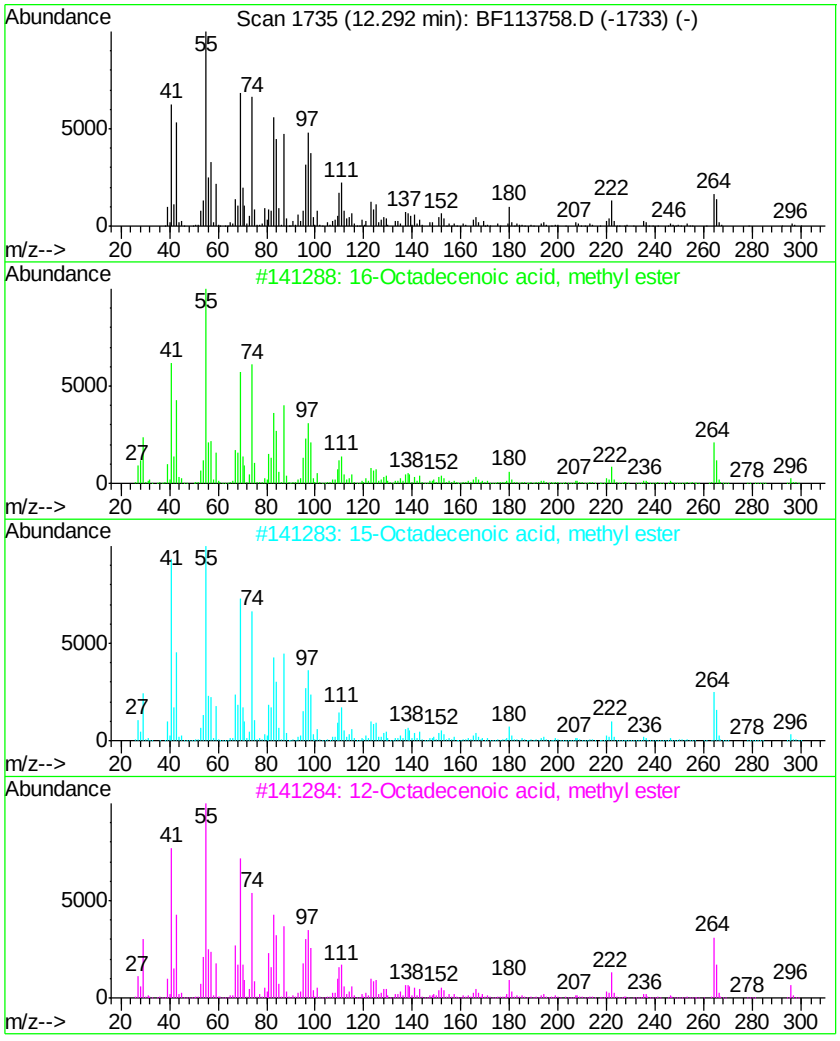
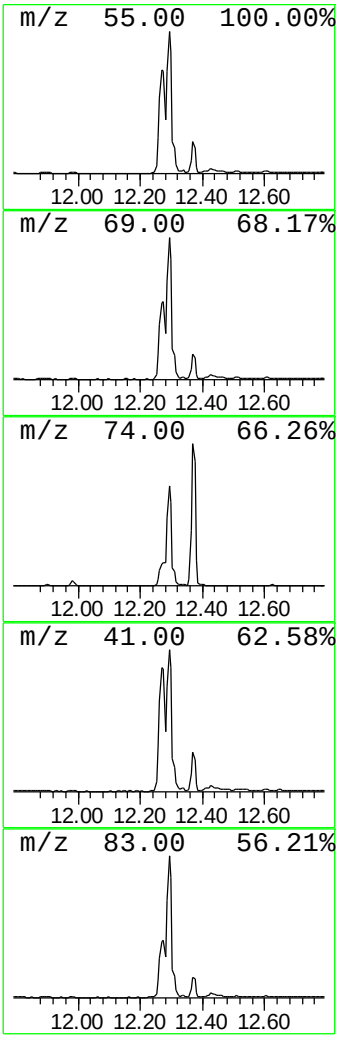
****

Peak Number 8 16-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	160.79 ng	5920220	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	96
2	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	96
3	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	94
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	94
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	93





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Acq On : 13 Apr 2019 00:50
Operator : JU/SJ
Sample : K2204-01 5X
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TR-04-041119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

****

Peak Number 9 7,10,13-Hexadecatrienoic ac... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.33	3.11 ng	114485	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,10,13-Hexadecatrienoic acid, m...	264	C17H28O2	056554-30-4	90
2	Spiro[cyclopropane-1,8'(1H')[3a....	204	C14H20O	452049-62-6	58
3	Cyclooctene, 3-ethenyl-	136	C10H16	002213-60-7	38
4	Cyclohexene, 3-ethenyl-	108	C8H12	000766-03-0	38
5	3-Heptadecen-5-yne, (Z)-	234	C17H30	074744-55-1	35