LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106543.D
Acq On : 18 Jun 2018 17:21
Operator : JU/SJ
Sample : J3505-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

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-BF061118.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	5.213	484	489	497	rVB	218686	286054	5.34%	0.742%
2	5.613	554	557	564	rBV	2844275	2758569	51.52%	7.154%
3	6.613	722	727	730	rBV	2728566	2755546	51.47%	7.146%
4	6.748	745	750	753	rBV	2864673	2738515	51.15%	7.102%
5	6.966	782	787	790	rBV	905289	702811	13.13%	1.823%
6	7.125	809	814	817	rVB	2461498	2199084	41.07%	5.703%
7	7.531	877	883	886	rBV	1917374	1910796	35.69%	4.956%
8	8.248	1001	1005	1008	rBV	1061112	846636	15.81%	2.196%
9	9.325	1181	1188	1191	rBV	3091932	2910588	54.36%	7.548%
10	9.713	1250	1254	1257	rBV	547785	422243	7.89%	1.095%
11	10.007	1300	1304	1307	rBV	1039290	875205	16.35%	2.270%
12	10.419	1372	1374	1377	rVB	91130	67626	1.26%	0.175%
13	10.801	1434	1439	1442	rBV	1783866	1622876	30.31%	4.209%
14	10.895	1452	1455	1461	rBV2	71149	82160	1.53%	0.213%
15	11.001	1470	1473	1477	rVB2	106737	86355	1.61%	0.224%
16	11.501	1554	1558	1561	rBV	797311	736551	13.76%	1.910%
17	11.795	1606	1608	1613	rVB	114542	96782	1.81%	0.251%
18	11.878	1618	1622	1625	rVB	2423049	2204986	41.18%	5.718%
19	12.572	1735	1740	1741	rBV	3834626	4633450	86.54%	12.017%
20	12.595	1741	1744	1749	rVV2	4223074	5353985	100.00%	13.885%
21	12.636	1749	1751	1753	rVV2	68486	58718	1.10%	0.152%
22	12.666	1753	1756	1760	rVB	1173622	982821	18.36%	2.549%
23	13.083	1823	1827	1831	rBV	2188313	2153574	40.22%	5.585%
24	13.319	1861	1867	1870	rVV2	135884	160201	2.99%	0.415%
25	13.395	1876	1880	1882	rBV	121853	107510	2.01%	0.279%
26	13.972	1975	1978	1985	rBV	168254	181990	3.40%	0.472%
27	14.072	1992	1995	2000	rBV	90206	83369	1.56%	0.216%
28	14.154	2006	2009	2013	rVB	756746	724190	13.53%	1.878%
29	15.030	2155	2158	2165	rVB2	44935	59240	1.11%	0.154%
30	15.707	2268	2273	2281	rBV	571618	756579	14.13%	1.962%

Sum of corrected areas: 38559010

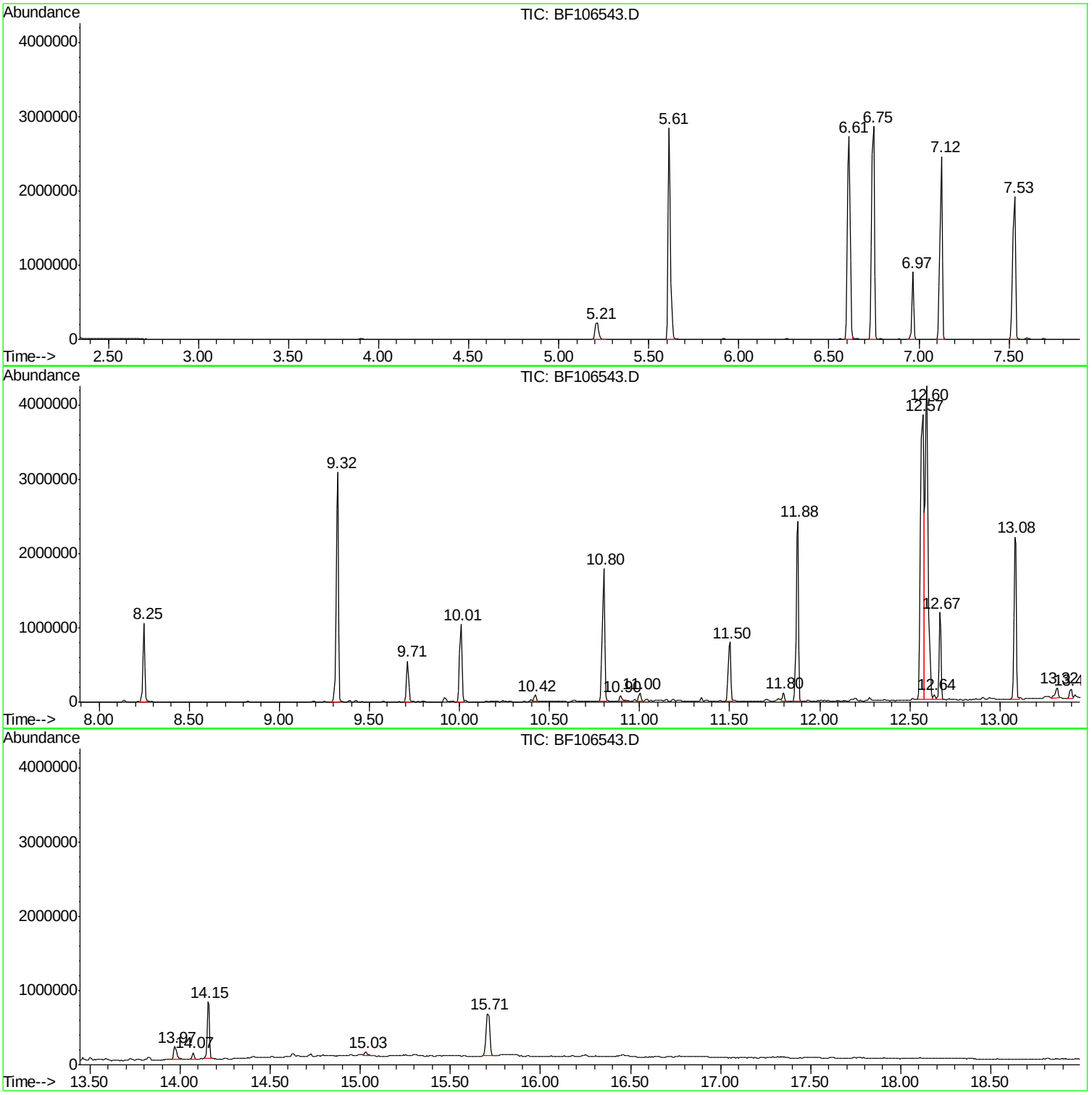
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106543.D
Acq On : 18 Jun 2018 17:21
Operator : JU/SJ
Sample : J3505-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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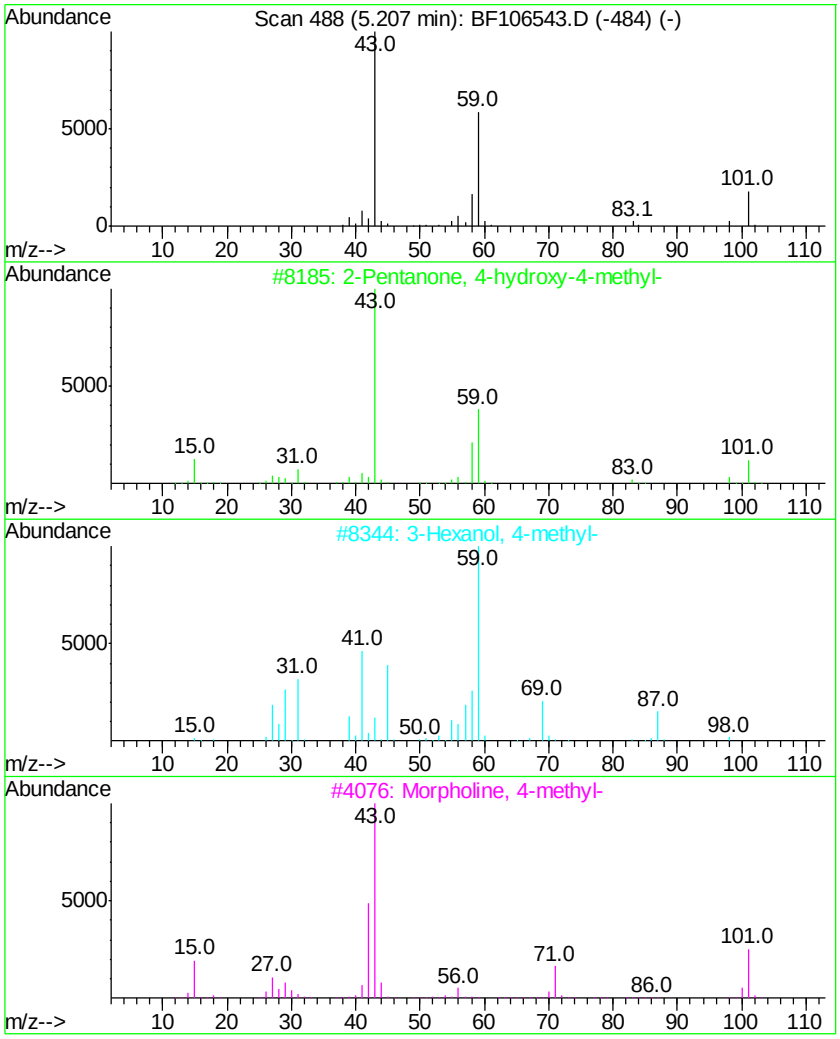
TIC Integration Parameters: LSCINT.P

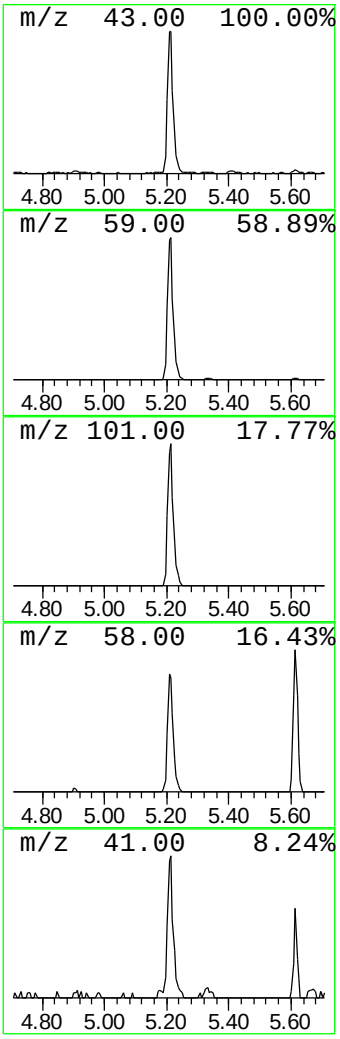
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	8.14 ng	286054	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9





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Operator : JU/SJ
Sample : J3505-02
Misc :
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Instrument : BNA_F
ClientSampleId : SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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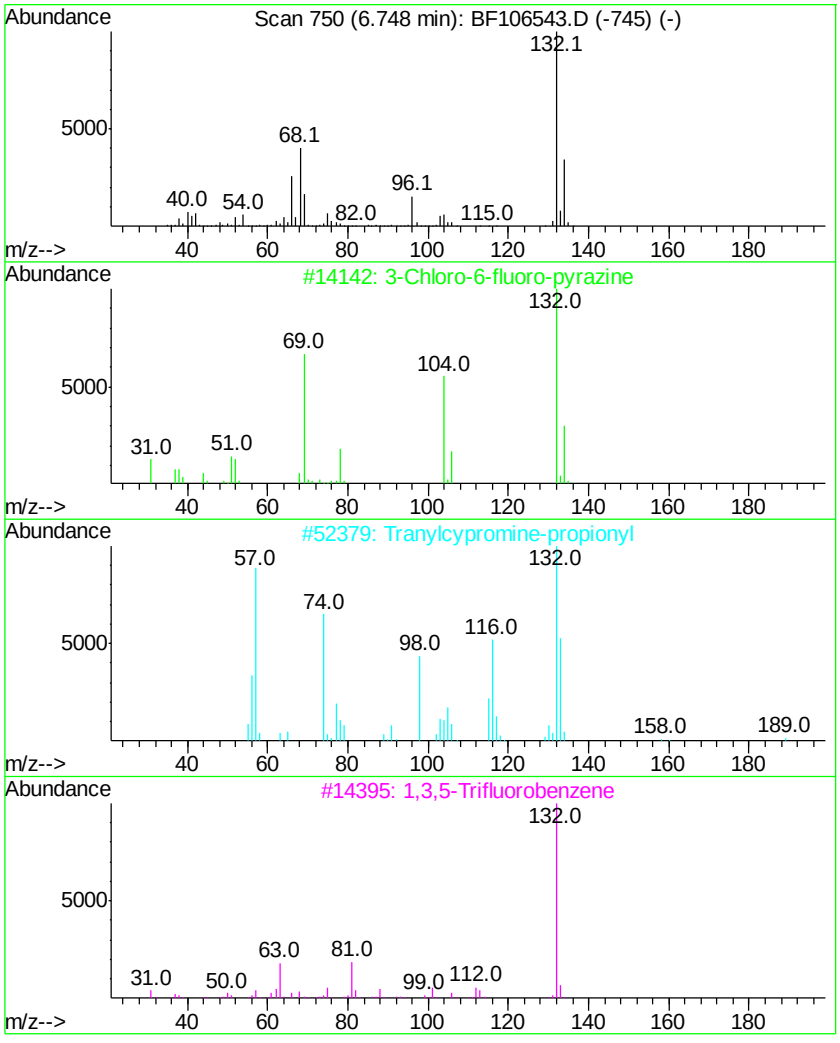
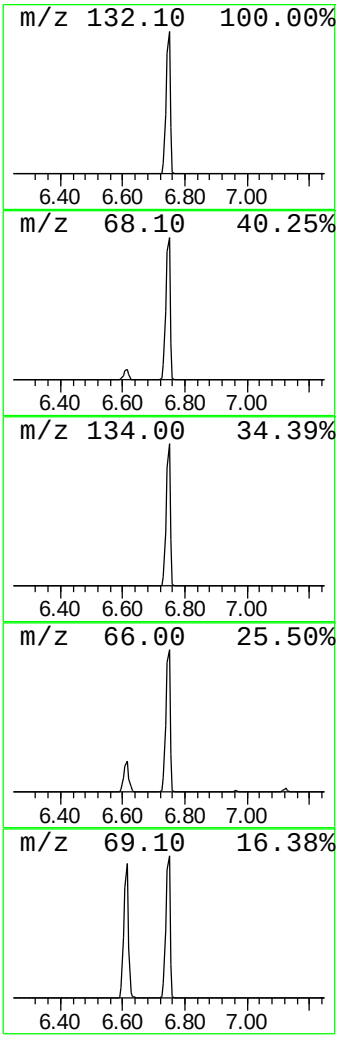
Peak Number 2 unknown6.75 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	77.93 ng	2738520	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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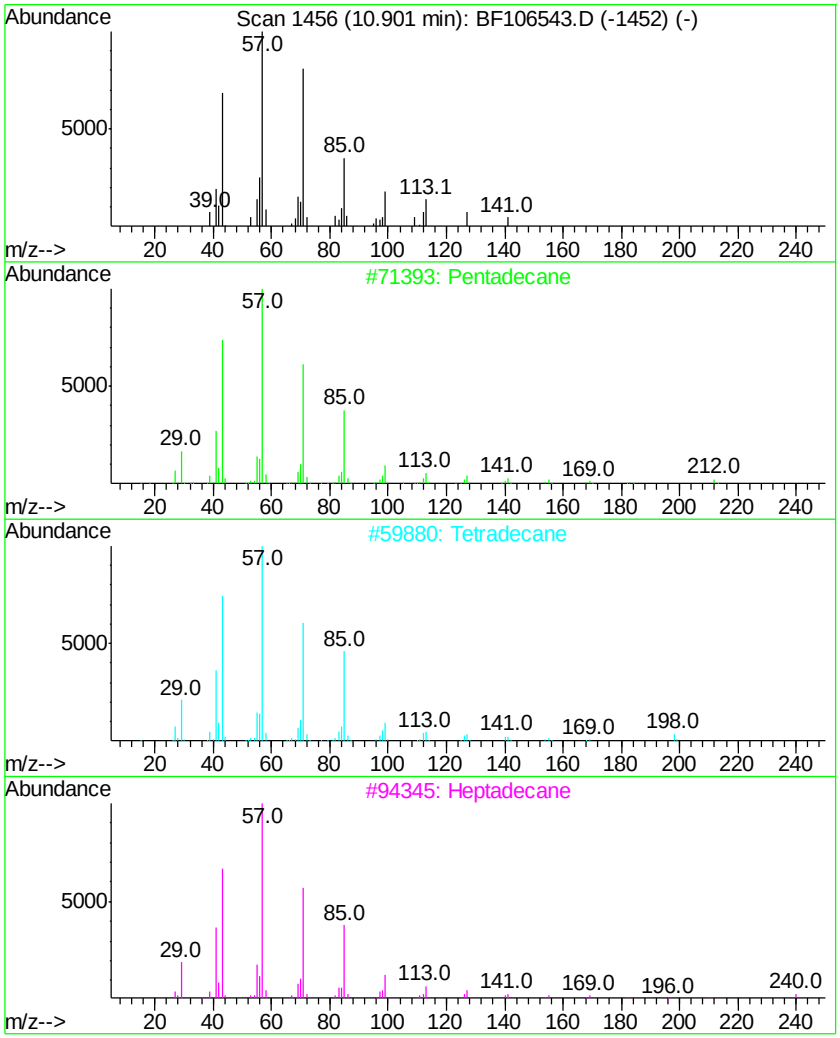
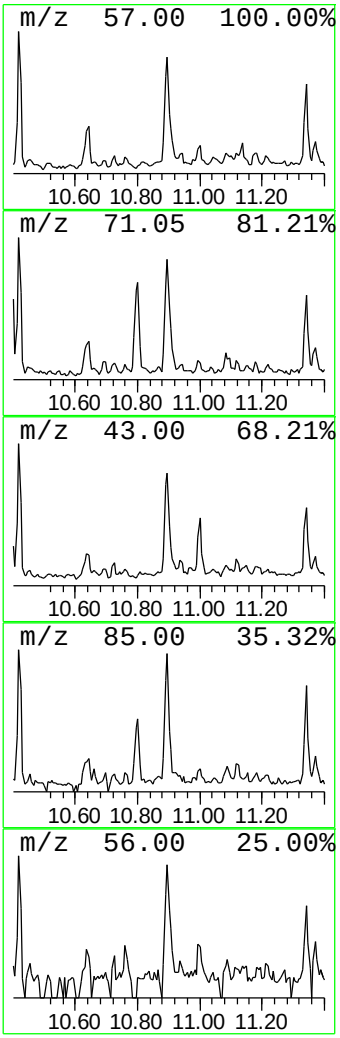
Peak Number 4 Pentadecane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.90	2.23 ng	82160	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Heptadecane	240	C17H36	000629-78-7	86
4	Tetracosane	338	C24H50	000646-31-1	83
5	Nonadecane	268	C19H40	000629-92-5	80





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Operator : JU/SJ
Sample : J3505-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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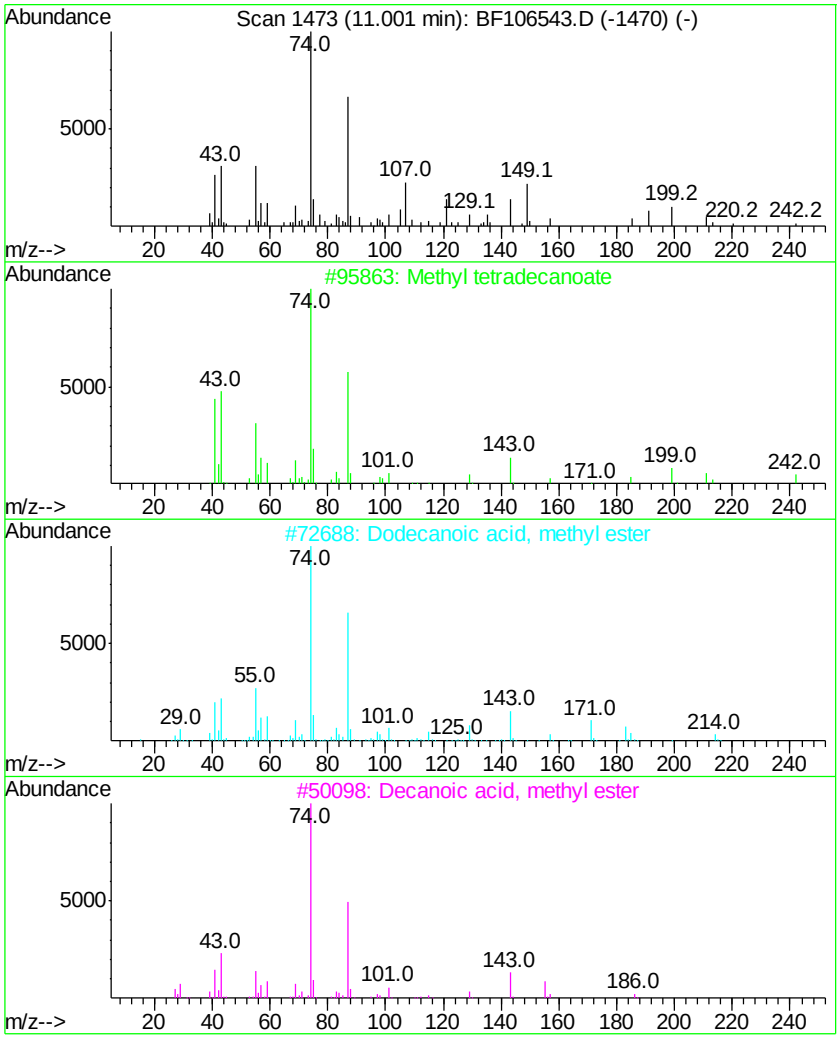
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

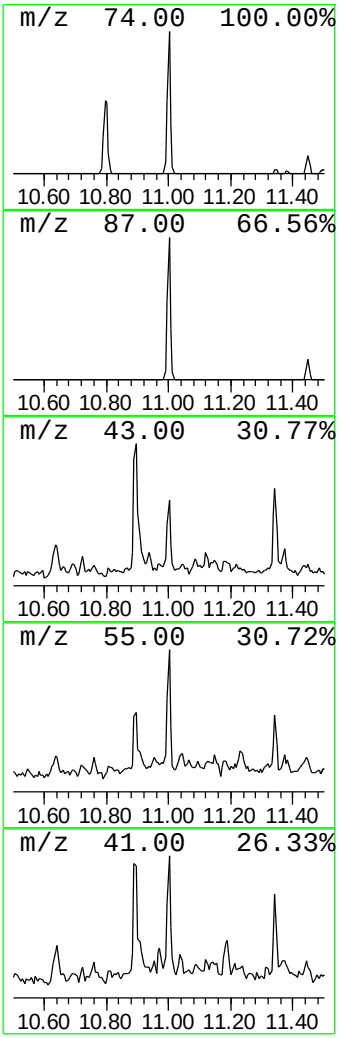
****

Peak Number 5 Methyl tetradecanoate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.00	2.34 ng	86355	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl tetradecanoate	242	C15H30O2	000124-10-7	81
2	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	58
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	52
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	52
5	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	52





Library Search Compound Report

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Sample : J3505-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.M
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TIC Library : C:\DATABASE\NIST11.L
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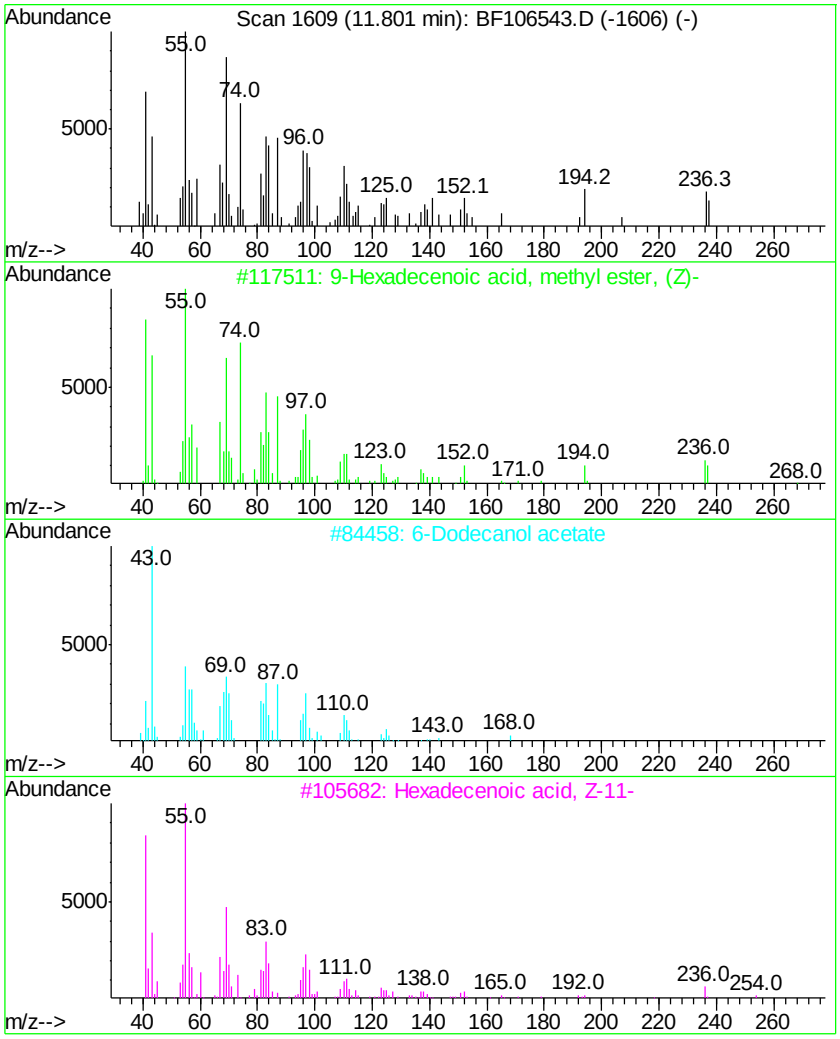
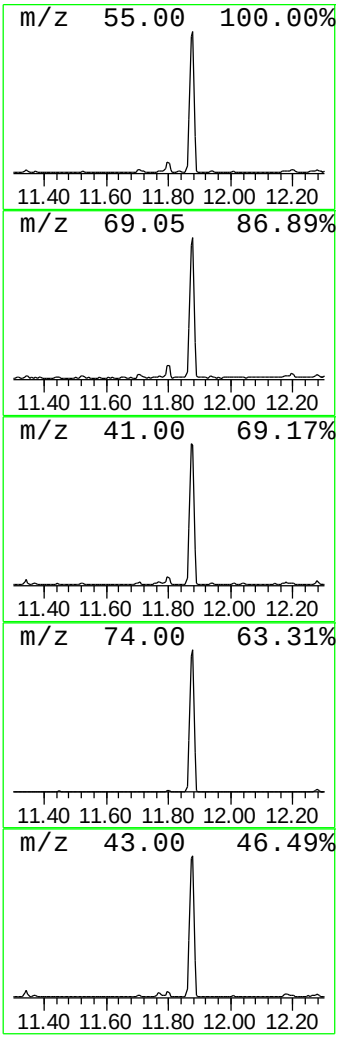
****

Peak Number 6 9-Hexadecenoic acid, methyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	2.63 ng	96782	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	87
2	6-Dodecanol acetate	228	C14H28O2	060826-23-5	50
3	Hexadecenoic acid, Z-11-	254	C16H30O2	002416-20-8	47
4	Palmitoleic acid	254	C16H30O2	000373-49-9	46
5	cis-9-Hexadecenoic acid	254	C16H30O2	1000333-19-5	46





Library Search Compound Report

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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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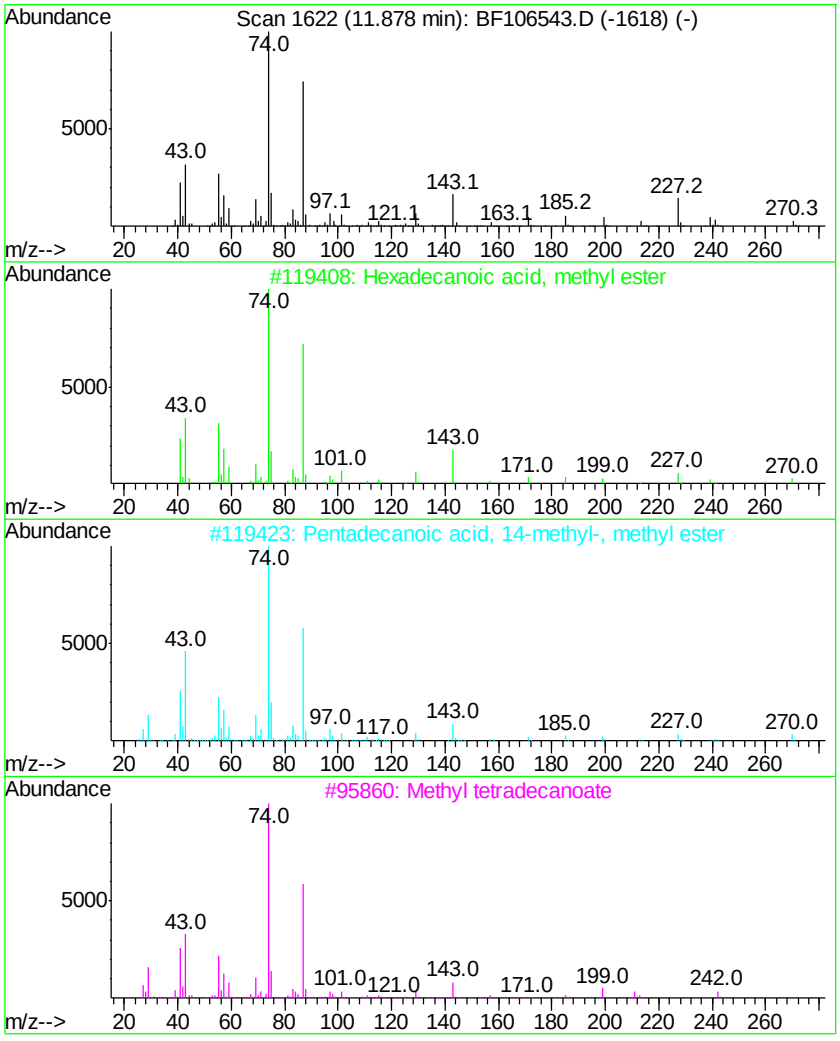
TIC Integration Parameters: LSCINT.P

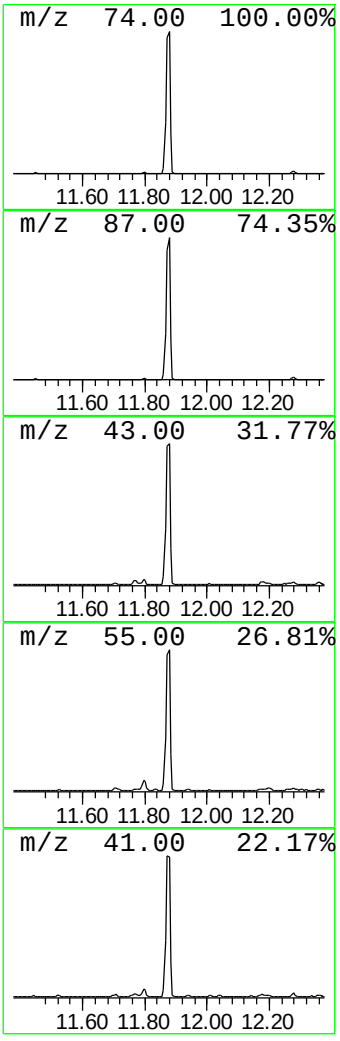
****

Peak Number 7 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	59.87 ng	2204990	Phenanthrene-d10	11.50

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	96
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	87





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

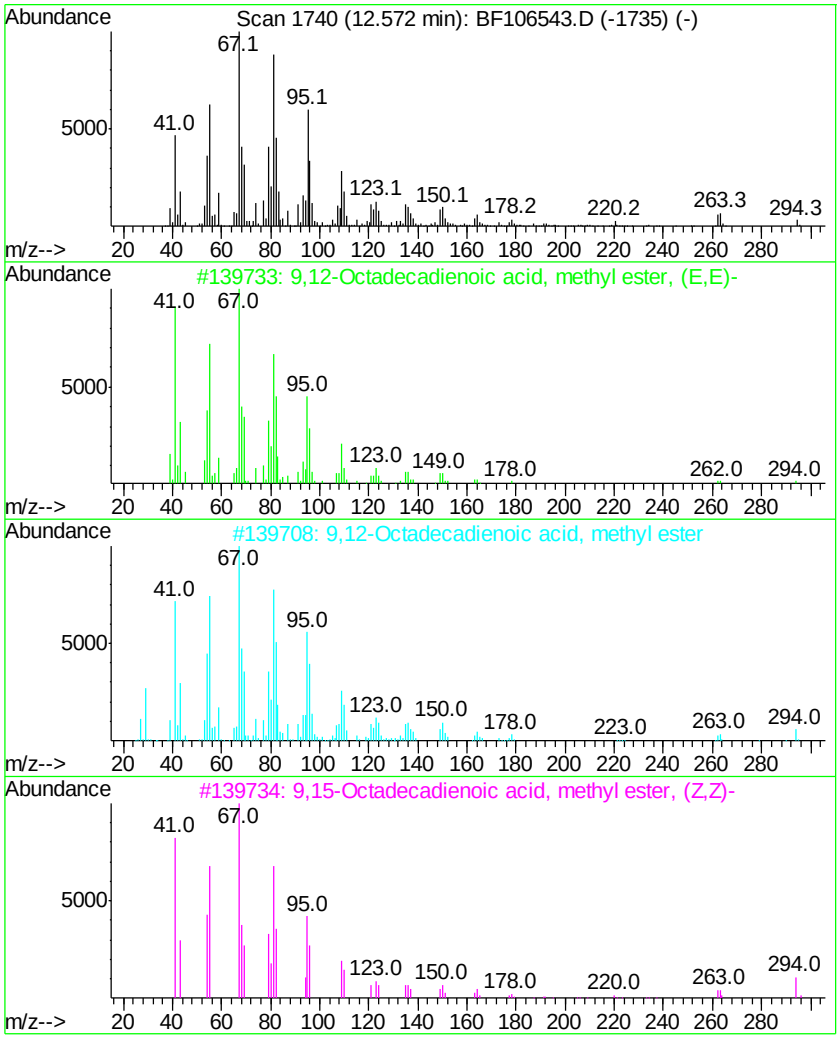
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

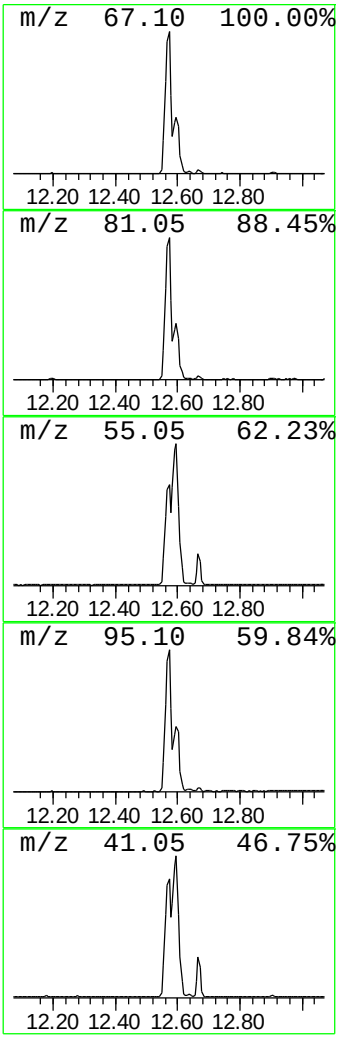
****

Peak Number 8 9,12-Octadecadienoic acid, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	125.82 ng	4633450	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
5	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99





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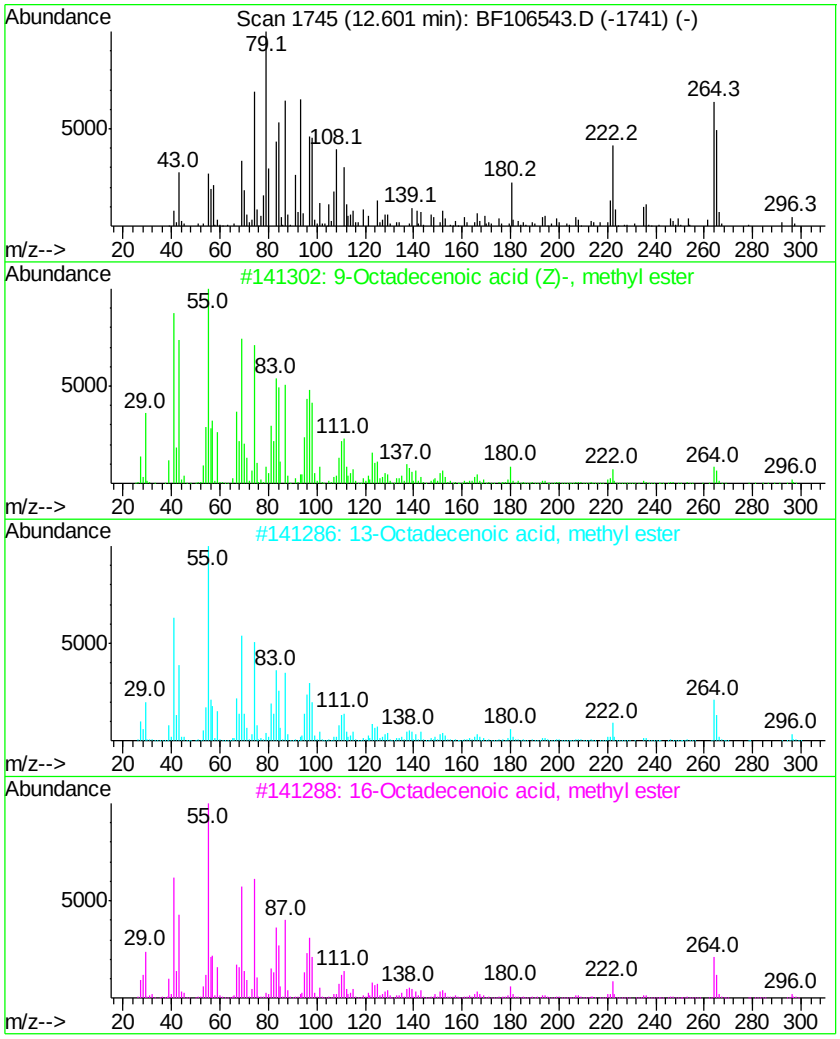
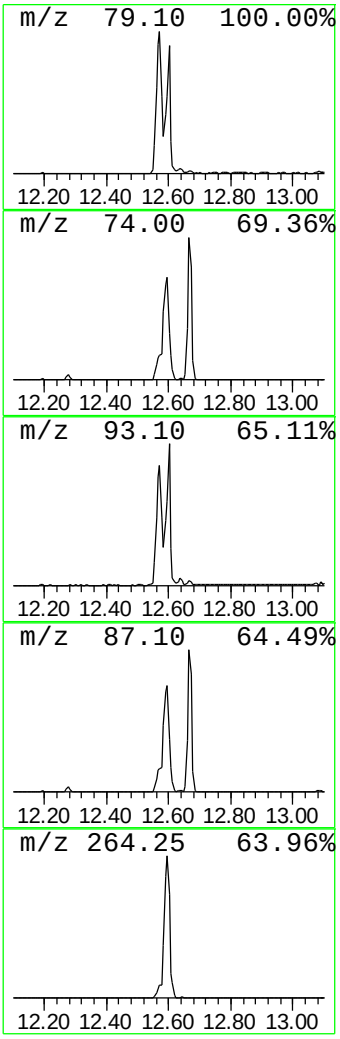
****

Peak Number 9 9-Octadecenoic acid (Z)-, m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	145.38 ng	5353990	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
2	13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	90
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	90
4	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	90
5	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1000333-58-3	74





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Instrument : BNA_F
ClientSampleId : SB-55-COMP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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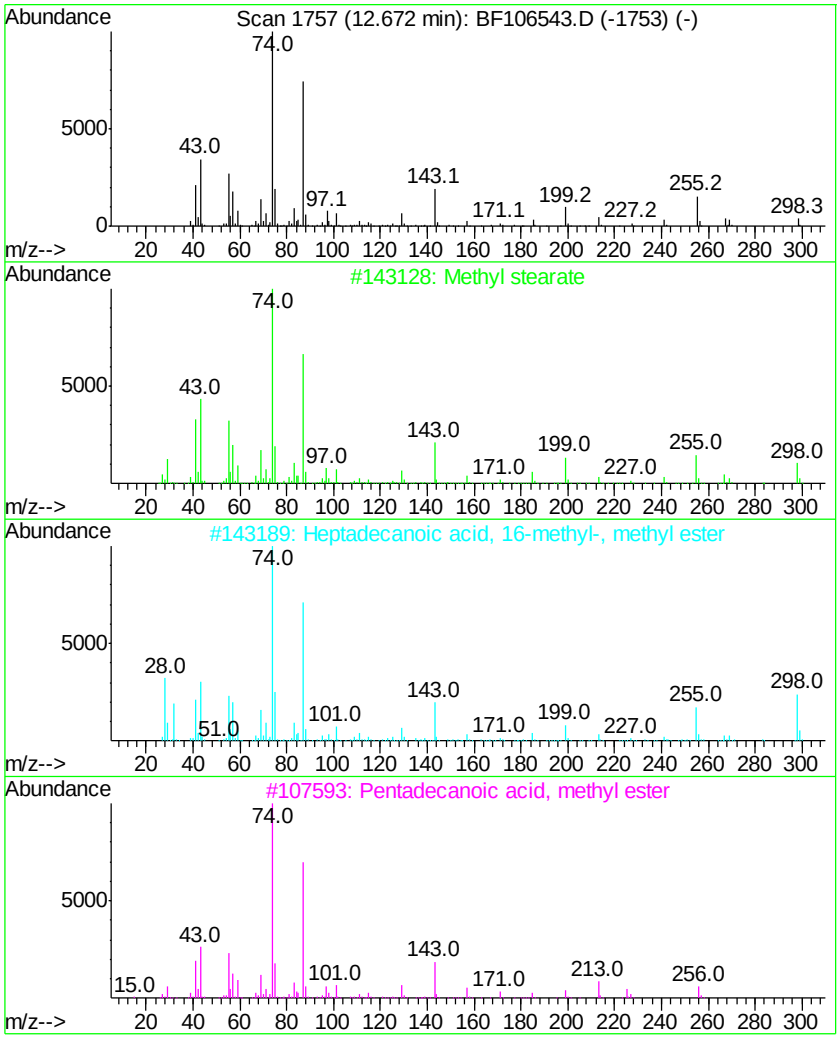
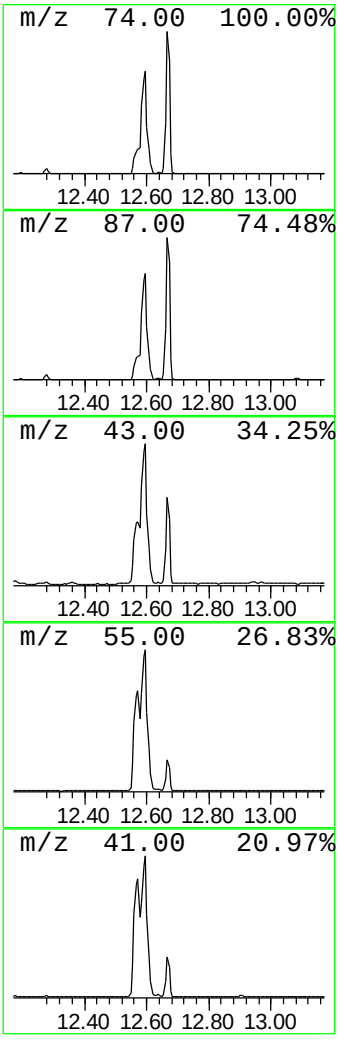
****

Peak Number 10 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.67	26.69 ng	982821	Phenanthrene-d10	11.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	97
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	93
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91





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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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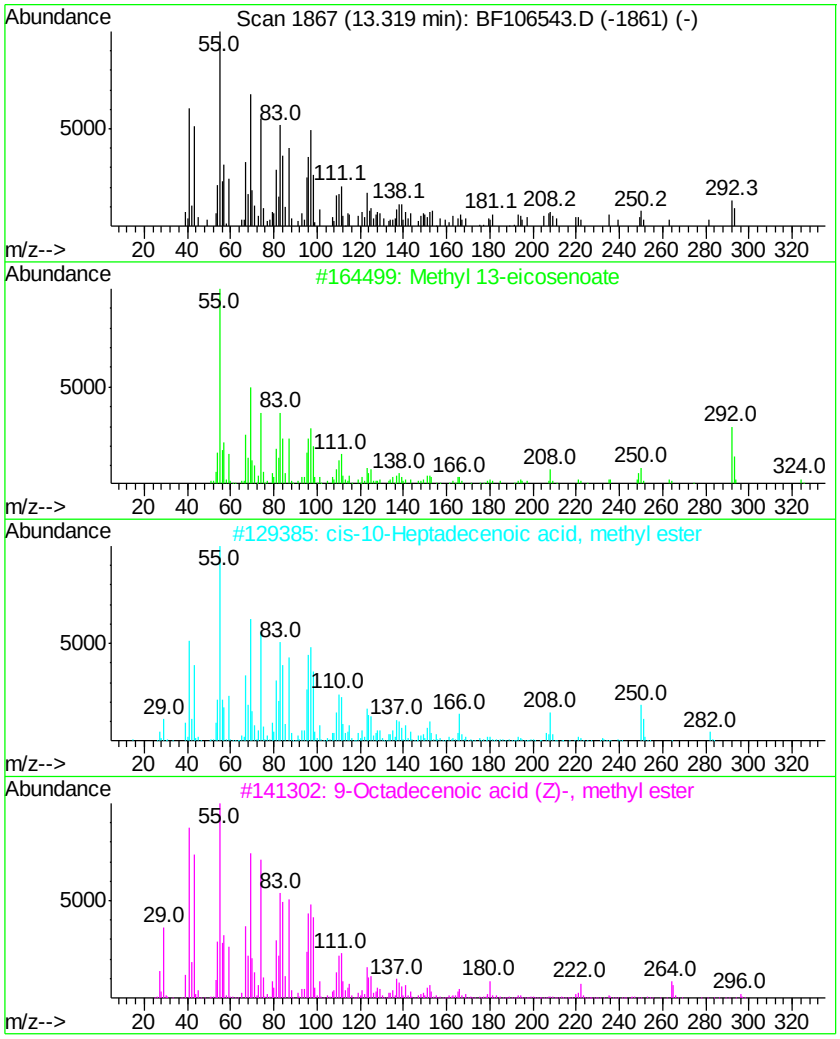
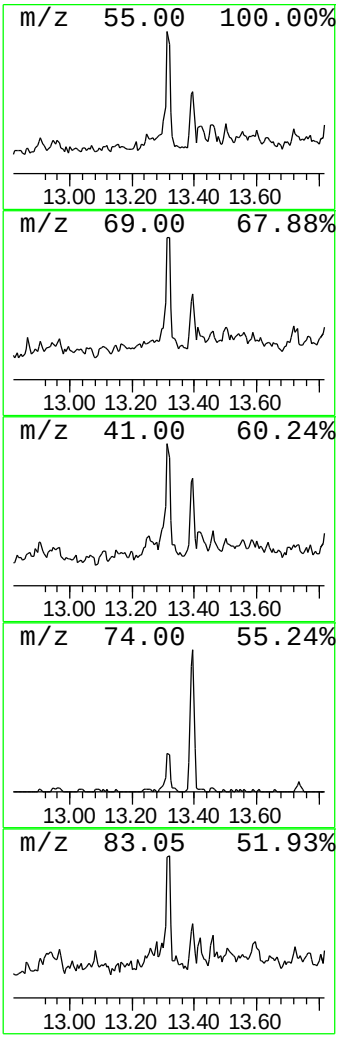
Peak Number 11 Methyl 13-eicosenoate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	4.42 ng	160201	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 13-eicosenoate	324	C21H40O2	1000336-48-4	87
2	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	87
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	81
4	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	70
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106543.D
Acq On : 18 Jun 2018 17:21
Operator : JU/SJ
Sample : J3505-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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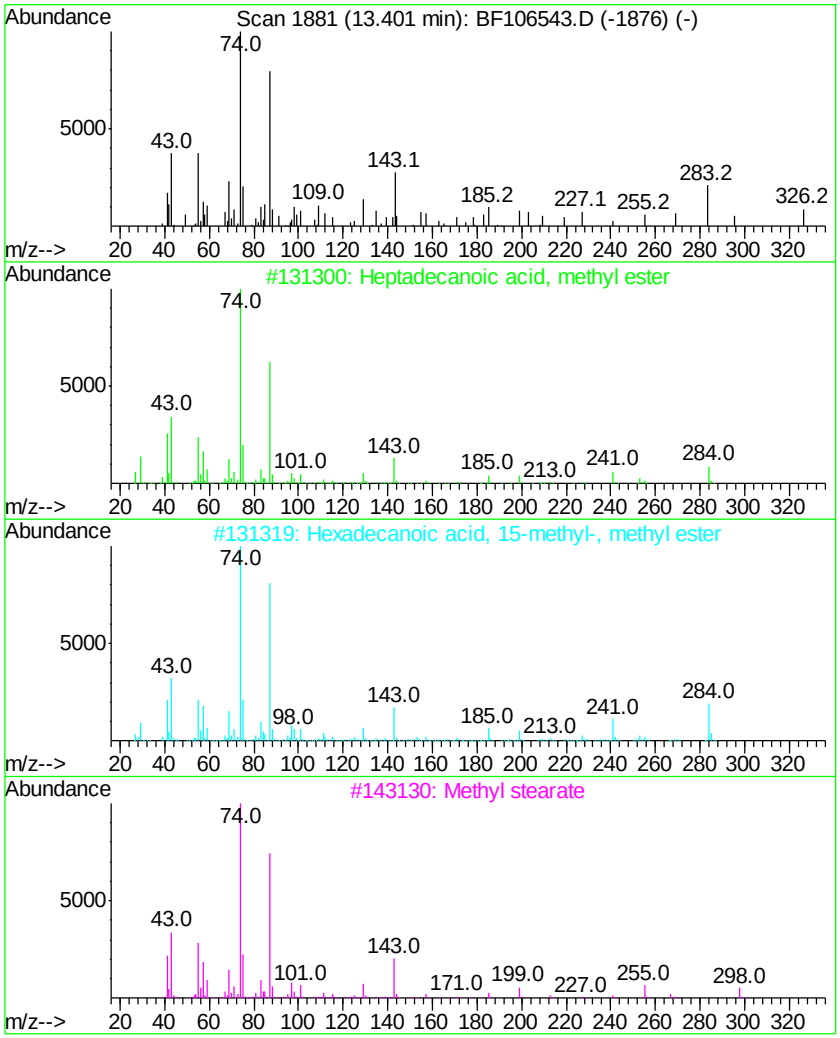
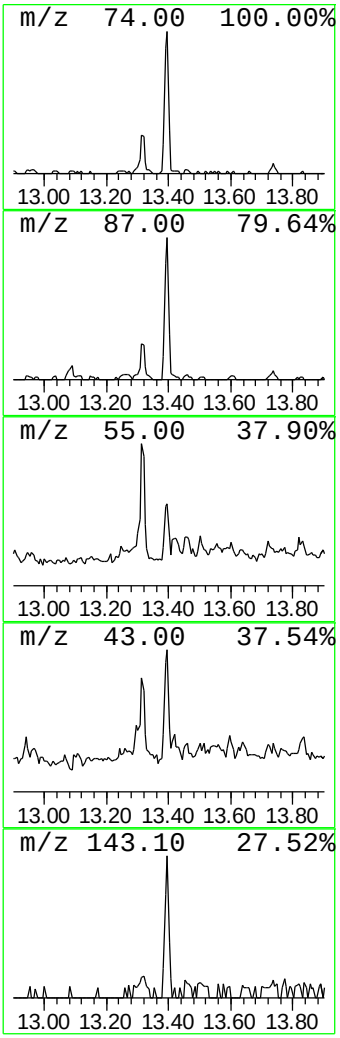
Peak Number 12 Heptadecanoic acid, methyl ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.40	2.97 ng	107510	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	94
2	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	93
3	Methyl stearate	298	C19H38O2	000112-61-8	87
4	Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	86
5	Eicosanoic acid, methyl ester	326	C21H42O2	001120-28-1	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106543.D
Acq On : 18 Jun 2018 17:21
Operator : JU/SJ
Sample : J3505-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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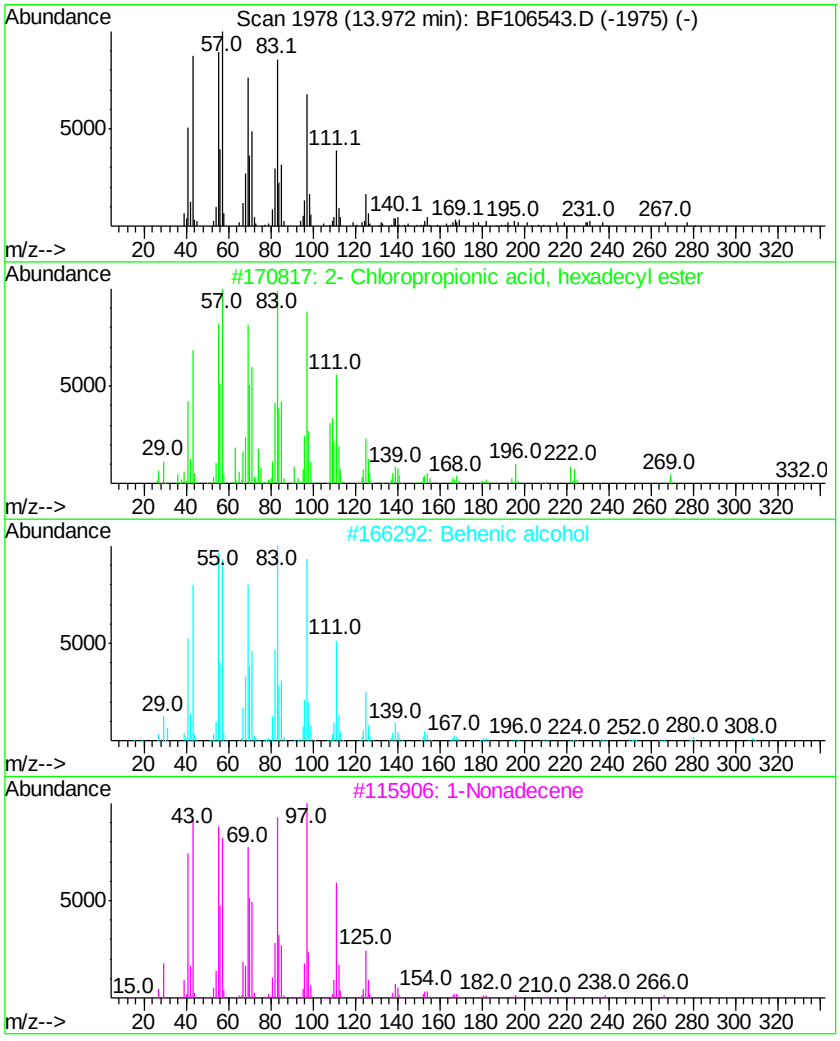
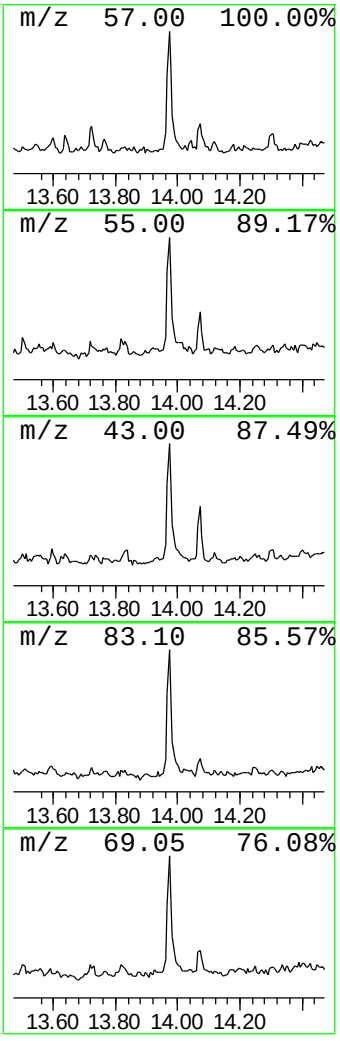
Peak Number 13 2- Chloropropionic acid, he... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	5.03 ng	181990	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	17-Pentatriacontene	491	C35H70	006971-40-0	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061818\
Data File : BF106543.D
Acq On : 18 Jun 2018 17:21
Operator : JU/SJ
Sample : J3505-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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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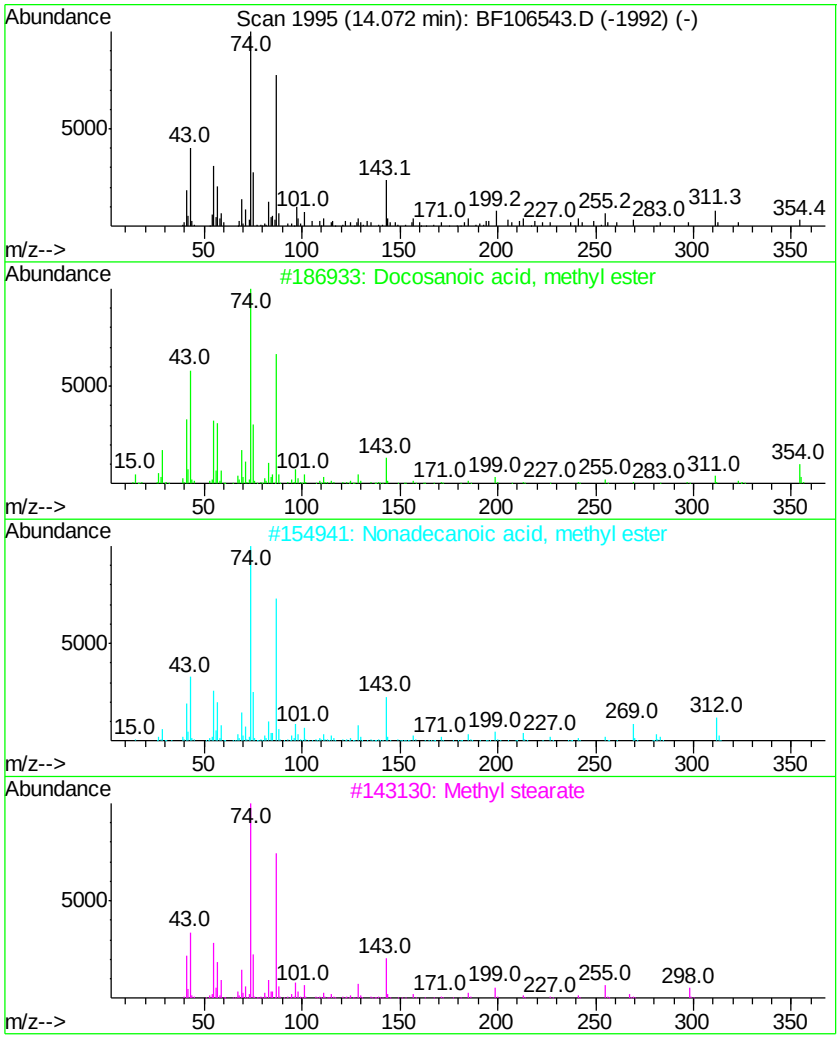
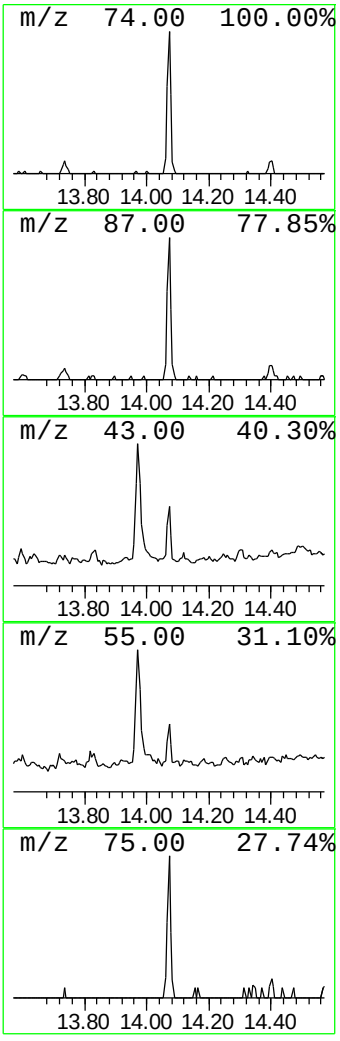
Peak Number 14 Docosanoic acid, methyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.07	2.30 ng	83369	Chrysene-d12	14.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosanoic acid, methyl ester	354	C23H46O2	000929-77-1	95
2	Nonadecanoic acid, methyl ester	312	C20H40O2	001731-94-8	94
3	Methyl stearate	298	C19H38O2	000112-61-8	86
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061818\
Data File : BF106543.D
Acq On : 18 Jun 2018 17:21
Operator : JU/SJ
Sample : J3505-02
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-55-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061118.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...	5.21	8.1	ng	286054	1	6.97	702811	20.0
unknown6.75	6.75	77.9	ng	2738520	1	6.97	702811	20.0
Pentadecane	10.90	2.2	ng	82160	4	11.50	736551	20.0
Methyl tetradecan...	11.00	2.3	ng	86355	4	11.50	736551	20.0
9-Hexadecenoic ac...	11.80	2.6	ng	96782	4	11.50	736551	20.0
Hexadecanoic acid...	11.88	59.9	ng	2204990	4	11.50	736551	20.0
9,12-Octadecadien...	12.57	125.8	ng	4633450	4	11.50	736551	20.0
9-Octadecenoic ac...	12.60	145.4	ng	5353990	4	11.50	736551	20.0
Methyl stearate	12.67	26.7	ng	982821	4	11.50	736551	20.0
Methyl 13-eicosen...	13.32	4.4	ng	160201	5	14.15	724190	20.0
Heptadecanoic aci...	13.40	3.0	ng	107510	5	14.15	724190	20.0
2- Chloropropioni...	13.97	5.0	ng	181990	5	14.15	724190	20.0
Docosanoic acid, ...	14.07	2.3	ng	83369	5	14.15	724190	20.0