LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118614.D
Acq On : 21 Jan 2020 1:59
Operator : CG/JU
Sample : L1004-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-101720

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-BF012020.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	2.216	13	22	28	rVB	2440994	3426303	38.75%	3.850%
2	5.110	506	514	522	rVB	1448071	1843150	20.84%	2.071%
3	5.510	577	582	585	rBV	8621594	8482686	95.93%	9.531%
4	6.510	746	752	755	rBV	8403443	8754510	99.01%	9.836%
5	6.651	772	776	780	rBV	8601158	8842440	100.00%	9.935%
6	6.881	812	815	819	rBV	2521628	2314517	26.18%	2.601%
7	7.039	838	842	846	rBV	7561839	7094327	80.23%	7.971%
8	7.439	905	910	913	rBV	5425909	5071286	57.35%	5.698%
9	8.163	1029	1033	1037	rBV	2844910	2583658	29.22%	2.903%
10	9.239	1211	1216	1220	rBV	9617491	8638517	97.69%	9.706%
11	9.627	1279	1282	1288	rBV	529823	466359	5.27%	0.524%
12	9.922	1326	1332	1335	rBV	3039282	2525824	28.56%	2.838%
13	10.710	1461	1466	1469	rBV	5383968	5039671	56.99%	5.662%
14	11.404	1580	1584	1587	rBV	2659748	2392311	27.05%	2.688%
15	11.427	1587	1588	1592	rVV	301454	195489	2.21%	0.220%
16	11.480	1593	1597	1600	rVB	143876	157697	1.78%	0.177%
17	11.804	1648	1652	1655	rVB	675802	580019	6.56%	0.652%
18	11.933	1671	1674	1681	rBV	827280	737346	8.34%	0.828%
19	12.021	1686	1689	1691	rBV3	115614	116257	1.31%	0.131%
20	12.486	1765	1768	1770	rBV	2116206	1924777	21.77%	2.163%
21	12.510	1770	1772	1778	rVB	2077352	1762174	19.93%	1.980%
22	12.592	1783	1786	1788	rBV	316340	298040	3.37%	0.335%
23	12.615	1788	1790	1793	rVB	614259	518017	5.86%	0.582%
24	12.715	1804	1807	1813	rBV2	216527	314054	3.55%	0.353%
25	12.845	1826	1829	1832	rVB	529472	476915	5.39%	0.536%
26	12.992	1850	1854	1857	rBV	9443189	8375387	94.72%	9.410%
27	13.886	2003	2006	2012	rBV	1636234	1783241	20.17%	2.004%
28	14.045	2029	2033	2036	rBV	2696458	2570238	29.07%	2.888%
29	15.515	2280	2283	2287	rVB	1448023	1716061	19.41%	1.928%

Sum of corrected areas: 89001271

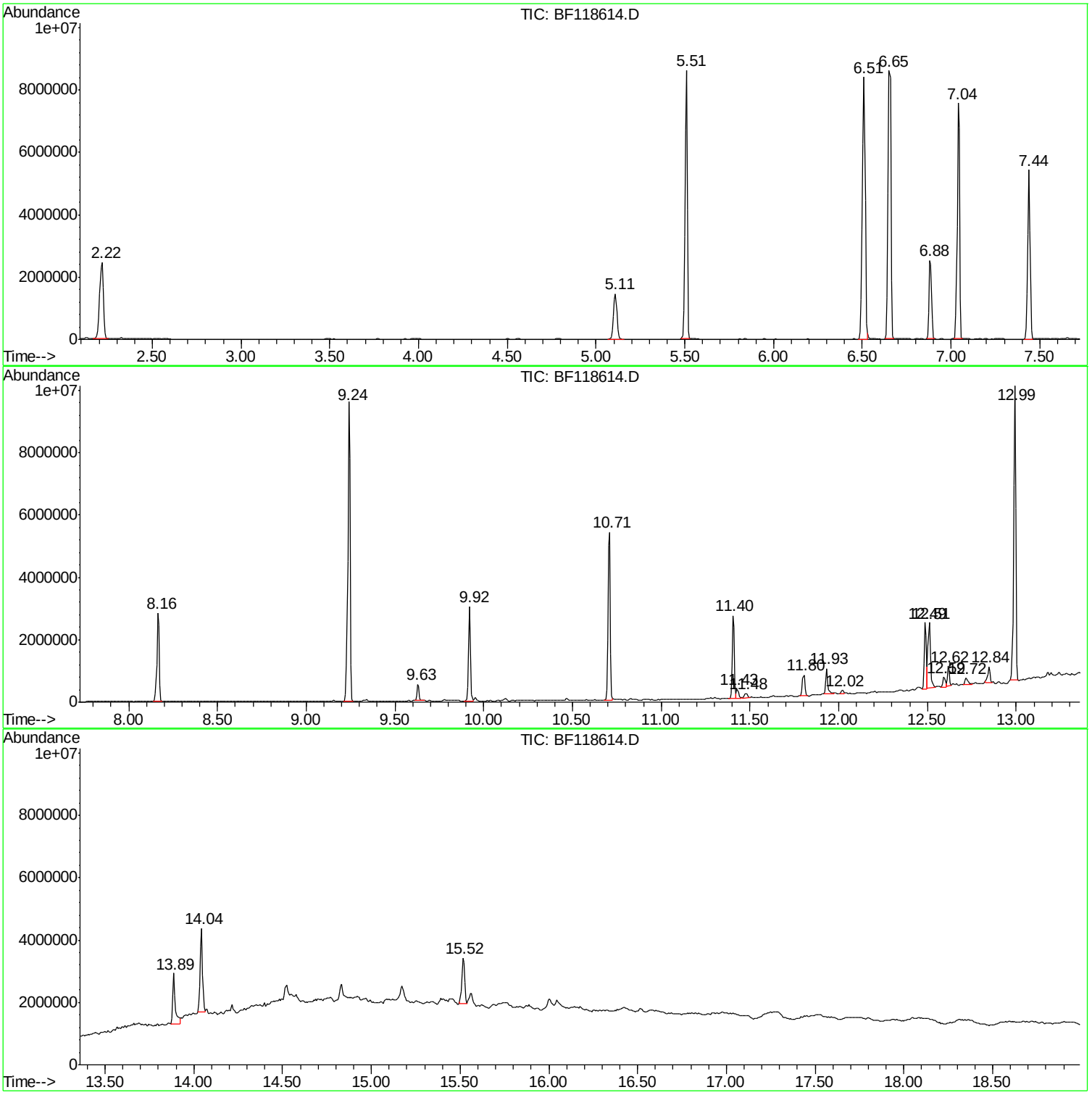
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118614.D
Acq On : 21 Jan 2020 1:59
Operator : CG/JU
Sample : L1004-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-101720

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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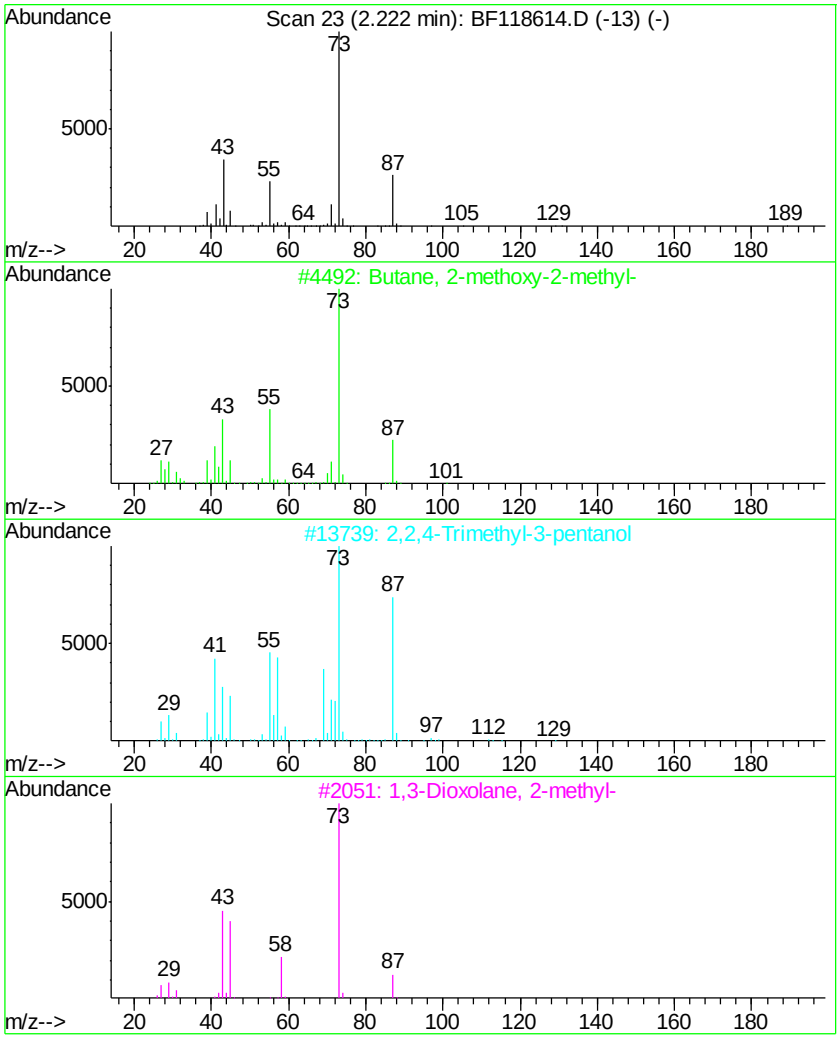
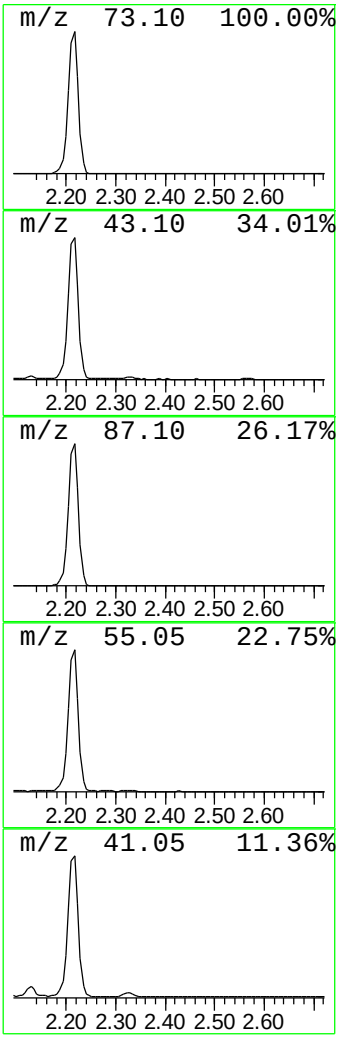
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	29.61 ng	3426300	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Data File : BF118614.D
Acq On : 21 Jan 2020 1:59
Operator : CG/JU
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Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-101720

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

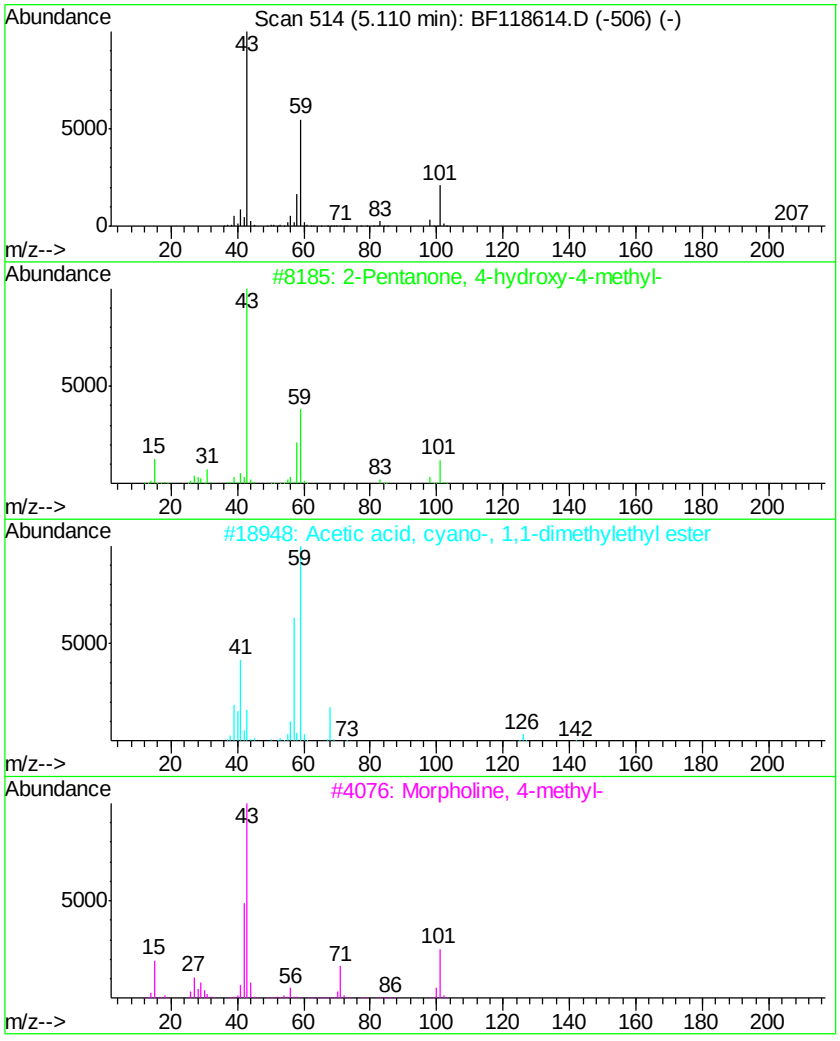
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

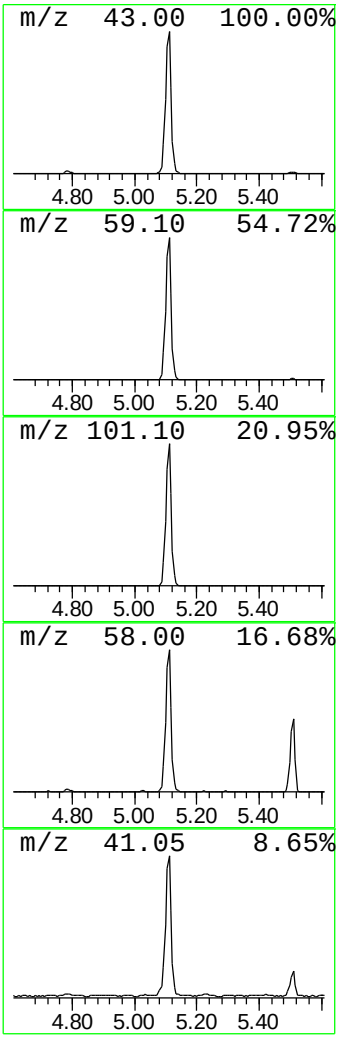
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	15.93 ng	1843150	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	N,N'-Bis(2-methyl-2-nitrosopenta...	258	C12H22N2O4	094514-30-4	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Library Search Compound Report

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Data File : BF118614.D
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Sample : L1004-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-101720

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

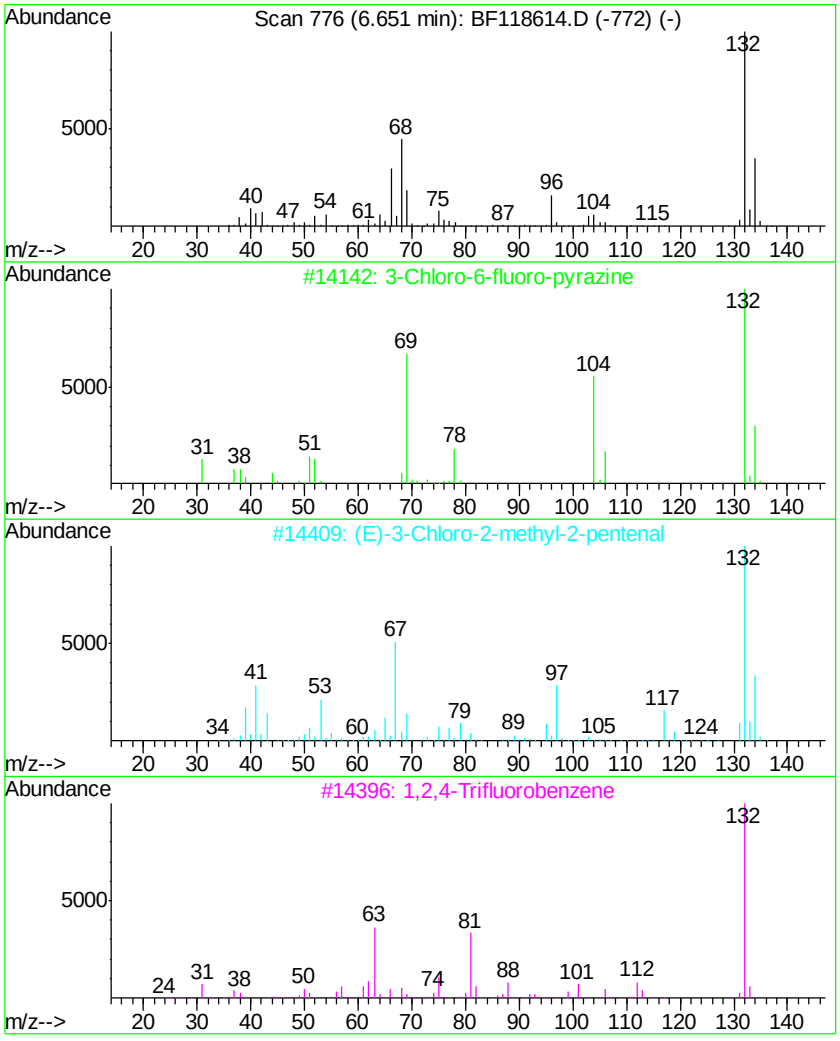
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

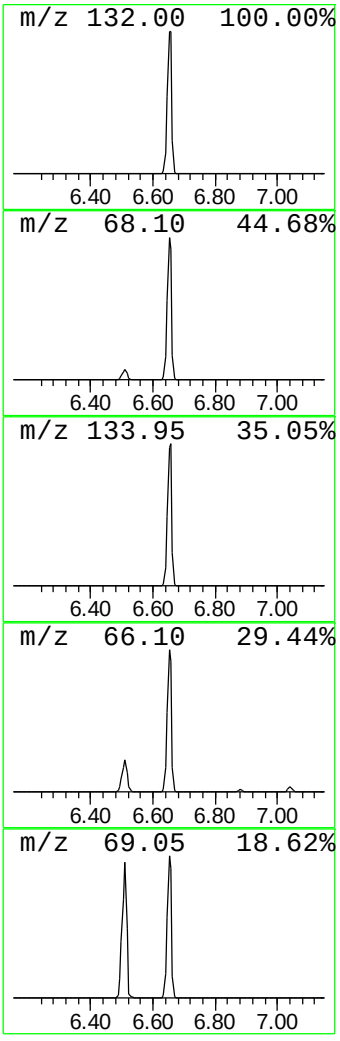
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	76.41 ng	8842440	1,4-Dichlorobenzene-d4	6.89

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	9
3	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
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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Operator : CG/JU
Sample : L1004-10
Misc :
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Instrument : BNA_F
ClientSampleId : BU-02-101720

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

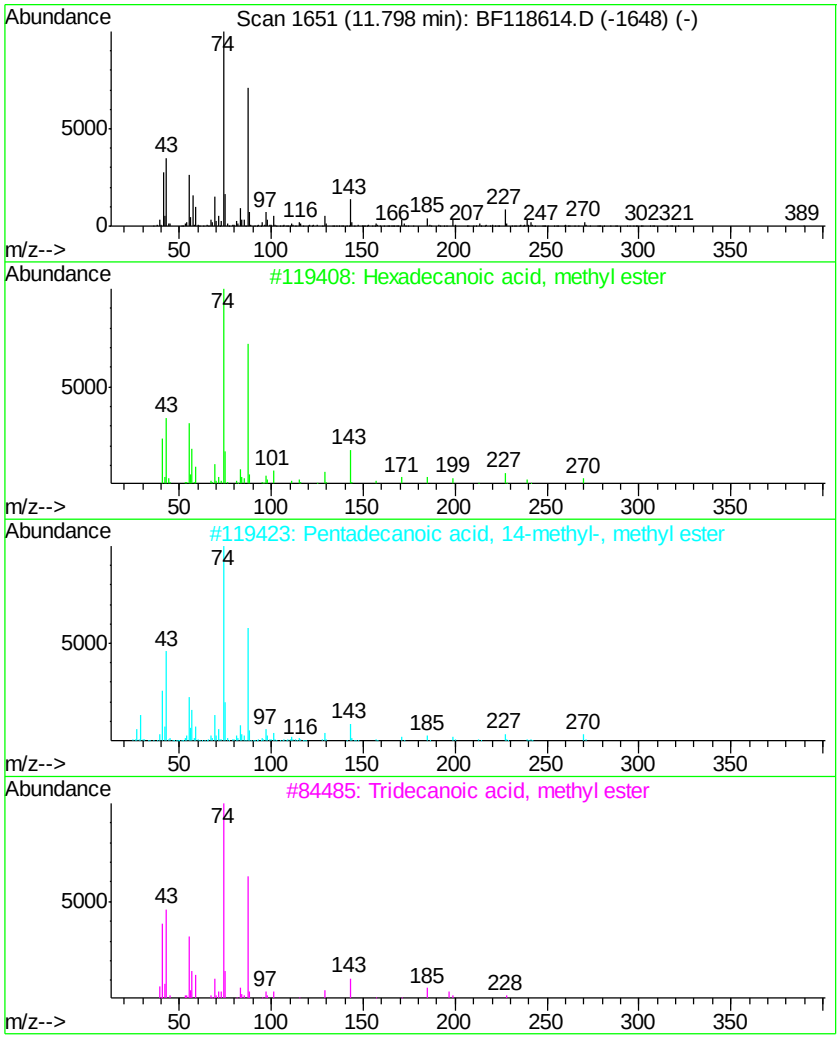
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

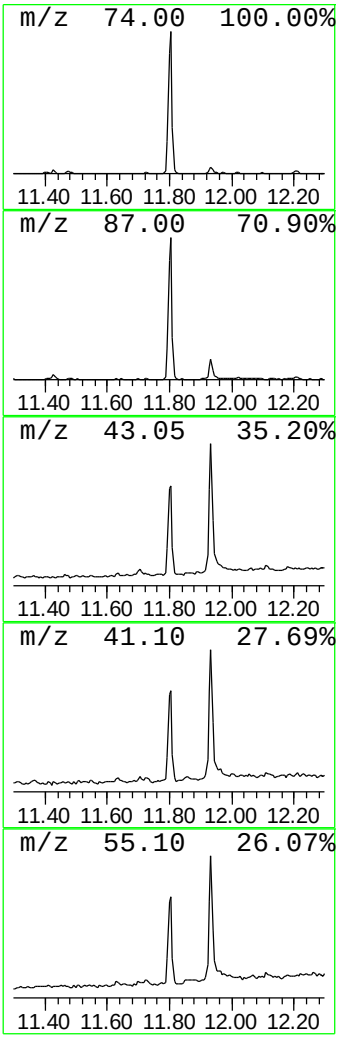
****

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.80	4.85 ng	580019	Phenanthrene-d10	11.40

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	89
4	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	87
5	Methyl stearate	298	C19H38O2	000112-61-8	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
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Acq On : 21 Jan 2020 1:59
Operator : CG/JU
Sample : L1004-10
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BU-02-101720

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

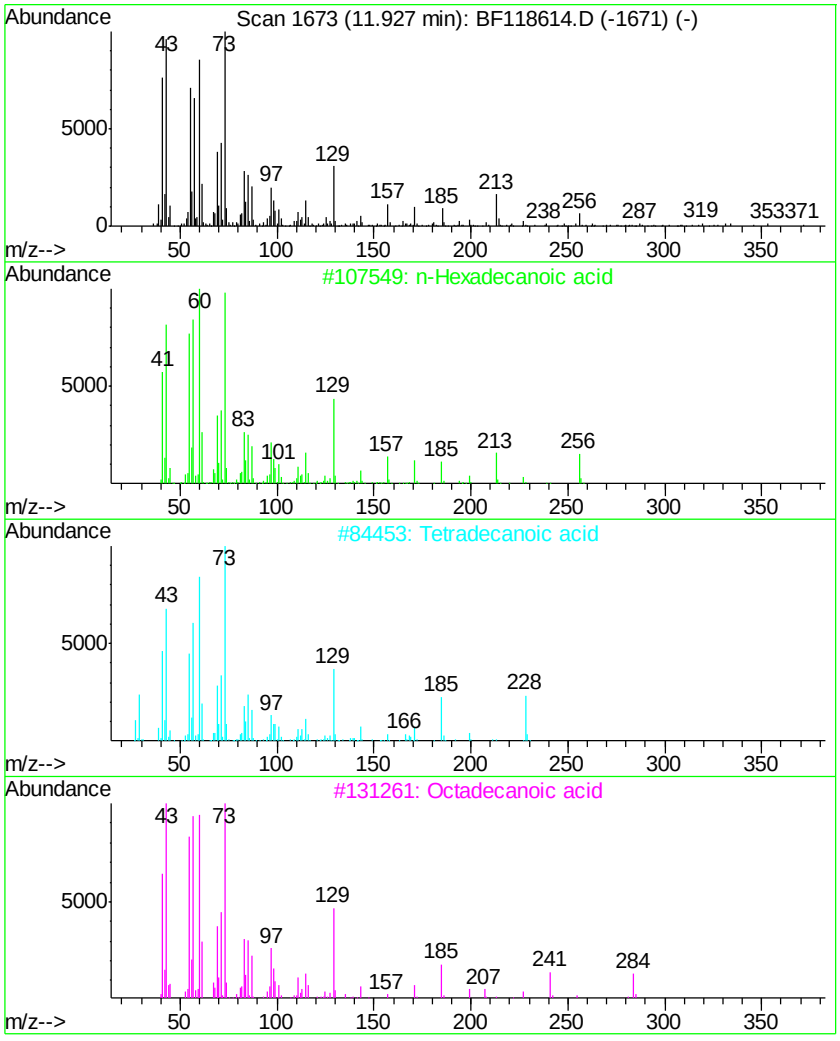
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

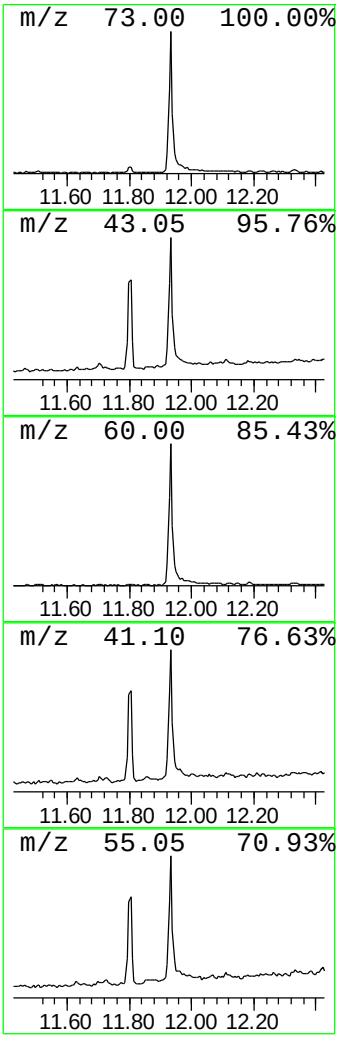
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	6.16 ng	737346	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Octadecanoic acid	284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Tridecanoic acid	214	C13H26O2	000638-53-9	89





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : BU-02-101720

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

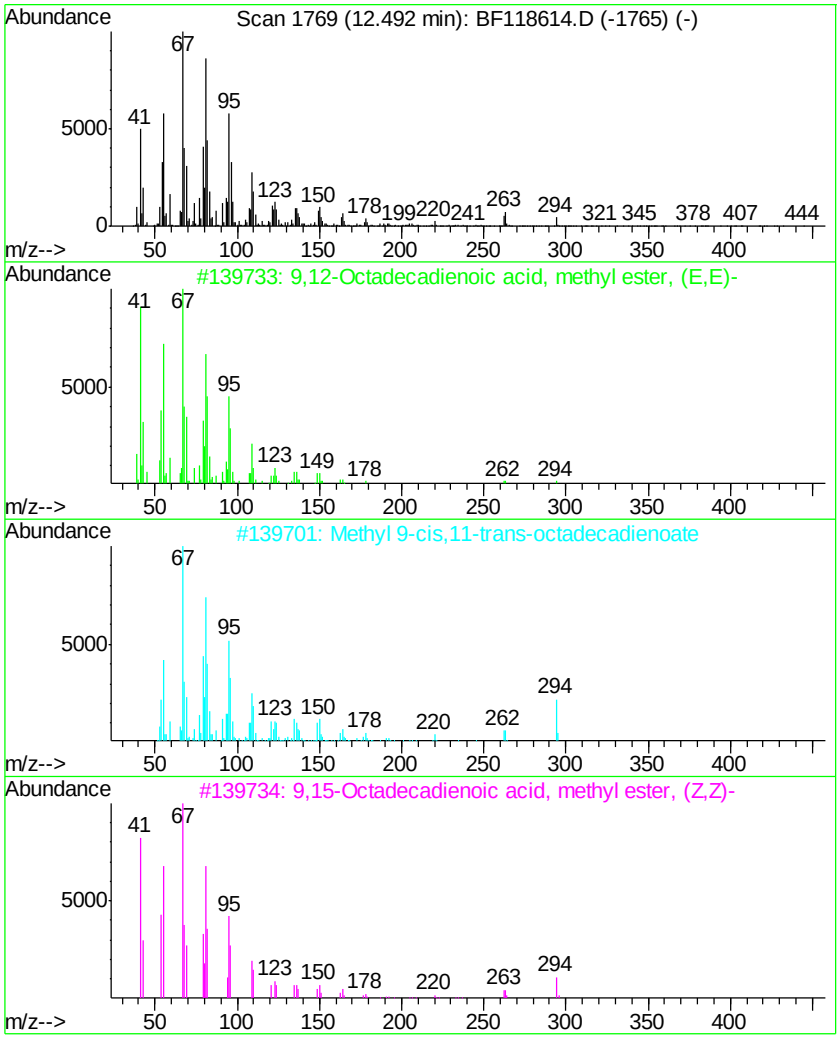
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

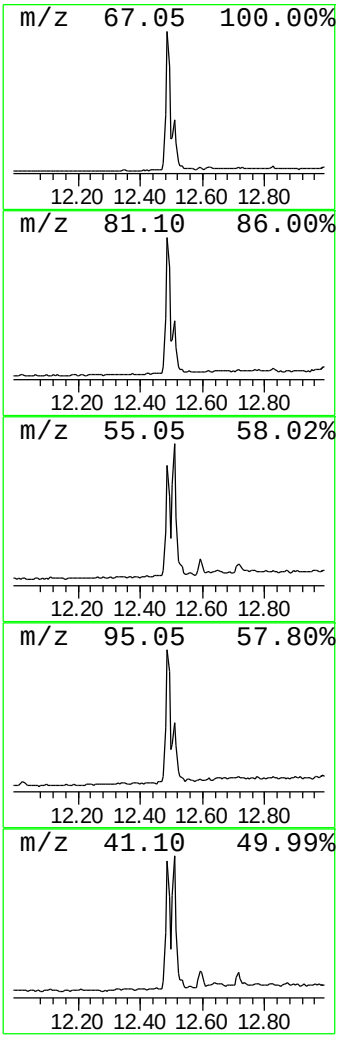
****

Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.49	16.09 ng	1924780	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methv...	294	C19H34O2	002566-97-4	99
2	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99
3	9,15-Octadecadienoic acid, methv...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
5	Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	98





Library Search Compound Report

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Misc :
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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

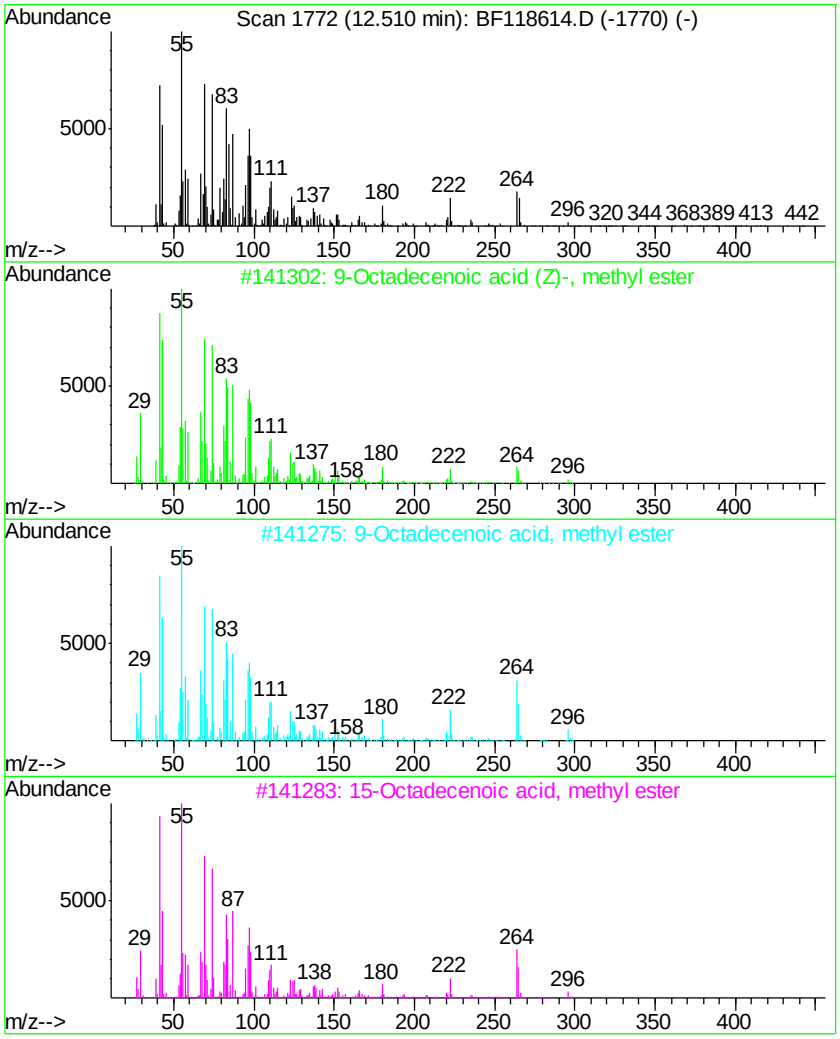
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

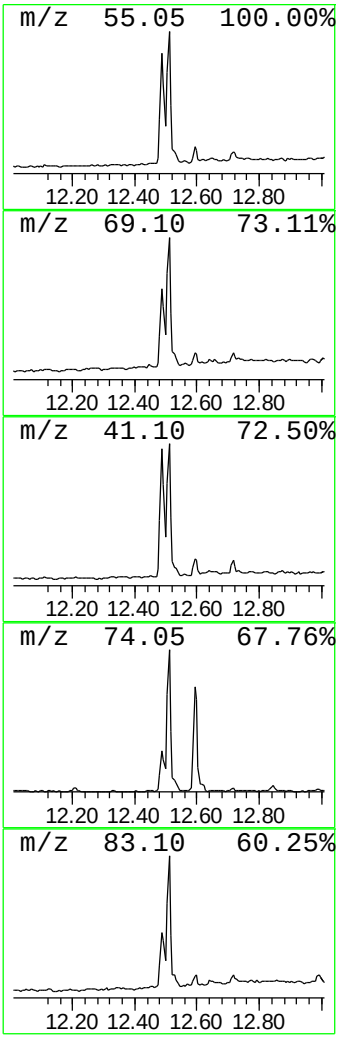
****

Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	14.73 ng	1762170	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	98
5	6-Octadecenoic acid, methyl ester	296	C19H36O2	052355-31-4	98





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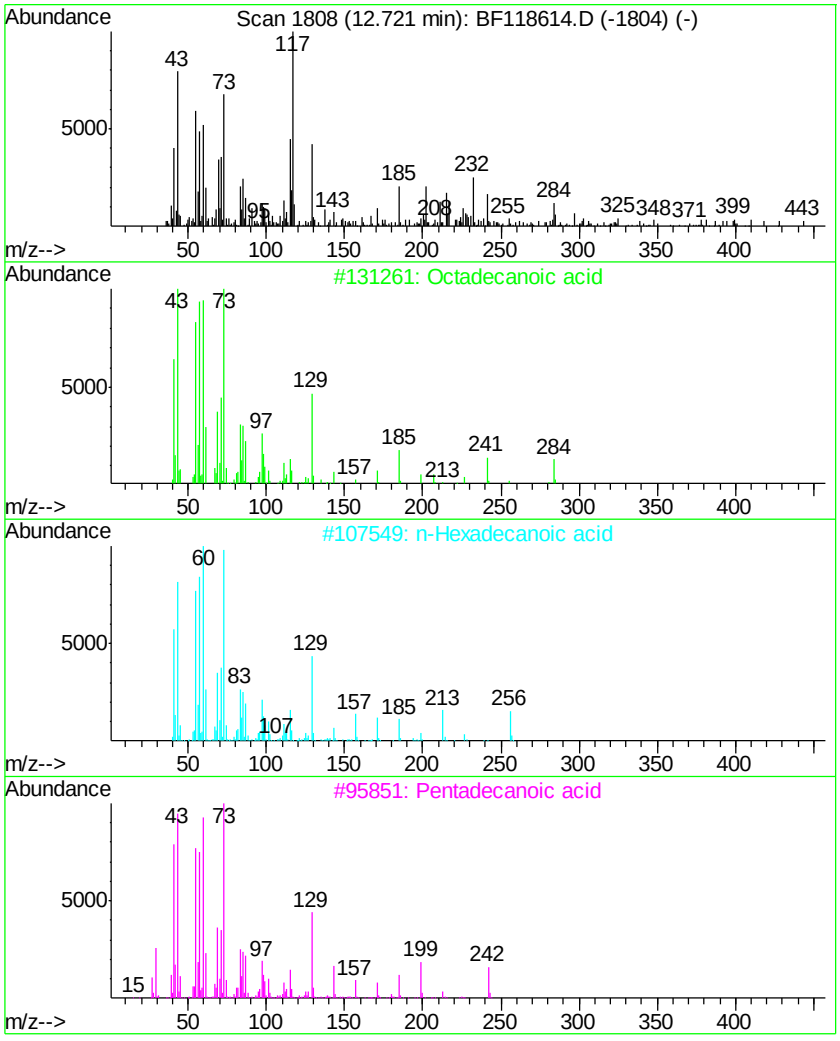
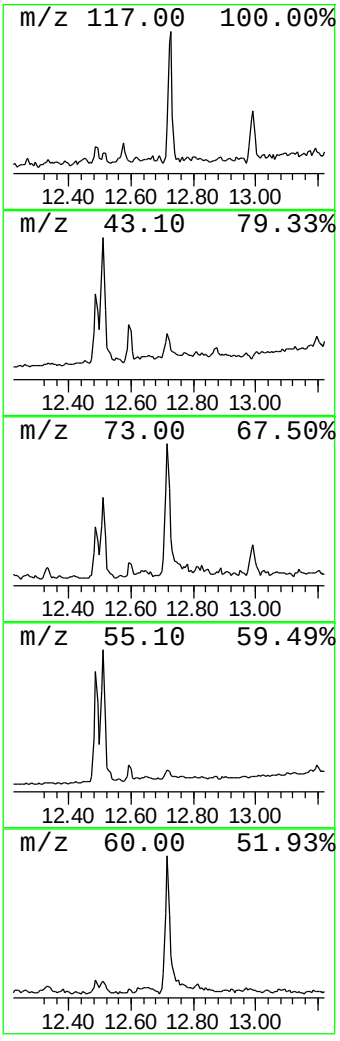
****

Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.63 ng	314054	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	68
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

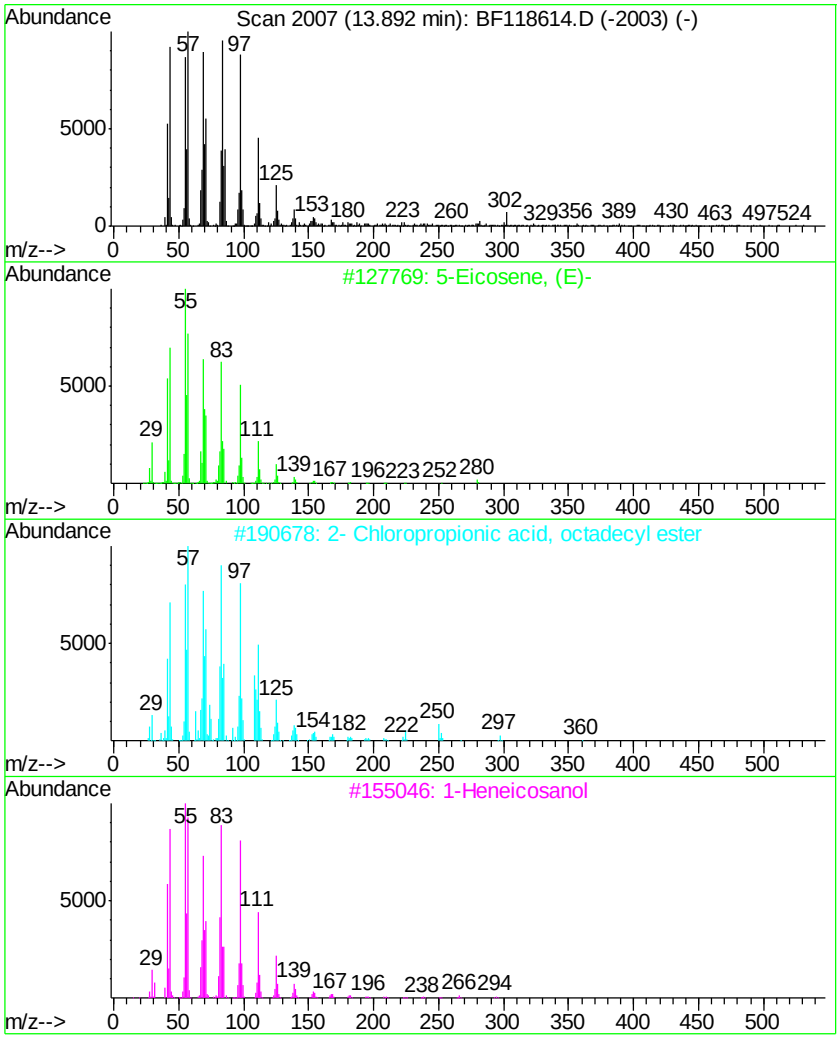
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

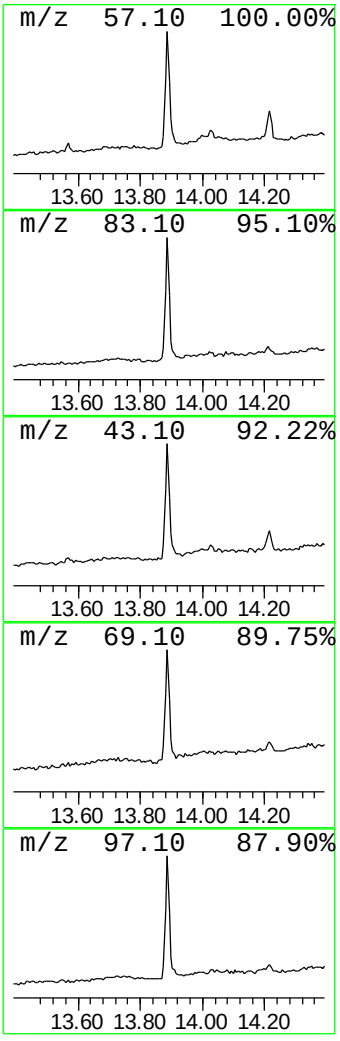
****

Peak Number 10 5-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	13.88 ng	1783240	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94





Tentatively Identified Compound (LSC) summary

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Instrument : BNA_F
ClientSampleId : BU-02-101720

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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
Butane, 2-methoxy...	2.22	29.6	ng	3426300	1	6.89	2314520	20.0
2-Pentanone, 4-hy...	5.11	15.9	ng	1843150	1	6.89	2314520	20.0
unknown6.65	6.65	76.4	ng	8842440	1	6.89	2314520	20.0
Hexadecanoic acid...	11.80	4.8	ng	580019	4	11.40	2392310	20.0
n-Hexadecanoic acid	11.93	6.2	ng	737346	4	11.40	2392310	20.0
9,12-Octadecadien...	12.49	16.1	ng	1924780	4	11.40	2392310	20.0
9-Octadecenoic ac...	12.51	14.7	ng	1762170	4	11.40	2392310	20.0
Octadecanoic acid	12.72	2.6	ng	314054	4	11.40	2392310	20.0
5-Eicosene, (E)-	13.89	13.9	ng	1783240	5	14.04	2570240	20.0