LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112944.D
Acq On : 8 Mar 2019 15:11
Operator : JU/SJ
Sample : K1783-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-2019-03-05

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-BF022719.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	5.340	548	553	569	rBV	2288956	2370096	36.48%	5.230%
2	6.357	722	726	734	rBV	1775179	1553031	23.91%	3.427%
3	6.498	745	750	753	rBV	4492287	4194244	64.56%	9.256%
4	6.728	785	789	793	rBV	1376726	1134170	17.46%	2.503%
5	6.887	812	816	819	rBV	4426644	3853103	59.31%	8.503%
6	7.293	879	885	897	rBV	2882938	3352173	51.60%	7.397%
7	8.010	1003	1007	1025	rBV	1449758	1421562	21.88%	3.137%
8	9.087	1185	1190	1205	rBV	5508028	5852205	90.08%	12.914%
9	9.757	1300	1304	1322	rBV	1551563	1629560	25.08%	3.596%
10	10.545	1433	1438	1467	rBV	3638913	3866568	59.52%	8.532%
11	11.239	1552	1556	1572	rVB	1688158	1816657	27.96%	4.009%
12	11.645	1621	1625	1633	rBV	423635	364945	5.62%	0.805%
13	12.304	1733	1737	1746	rBV4	30880	71358	1.10%	0.157%
14	12.427	1755	1758	1762	rBV	382970	345241	5.31%	0.762%
15	12.651	1792	1796	1800	rBV	1544362	1290815	19.87%	2.848%
16	12.822	1820	1825	1828	rBV	5847645	6496646	100.00%	14.336%
17	13.351	1912	1915	1919	rBV	910799	826396	12.72%	1.824%
18	13.863	1997	2002	2011	rBV	1710582	1946329	29.96%	4.295%
19	14.045	2029	2033	2039	rBV	80139	78965	1.22%	0.174%
20	14.345	2081	2084	2089	rVB	137060	118578	1.83%	0.262%
21	14.639	2130	2134	2138	rBV	186187	177467	2.73%	0.392%
22	14.710	2142	2146	2151	rVB	190843	186189	2.87%	0.411%
23	14.957	2184	2188	2196	rVB	178828	195889	3.02%	0.432%
24	15.263	2235	2240	2245	rBV	1089105	1544661	23.78%	3.409%
25	15.310	2245	2248	2257	rVB	194097	271430	4.18%	0.599%
26	15.716	2312	2317	2324	rVB	131162	198431	3.05%	0.438%
27	16.180	2391	2396	2405	rVB	92062	159143	2.45%	0.351%

Sum of corrected areas: 45315852

LSC Report - Integrated Chromatogram

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Misc :
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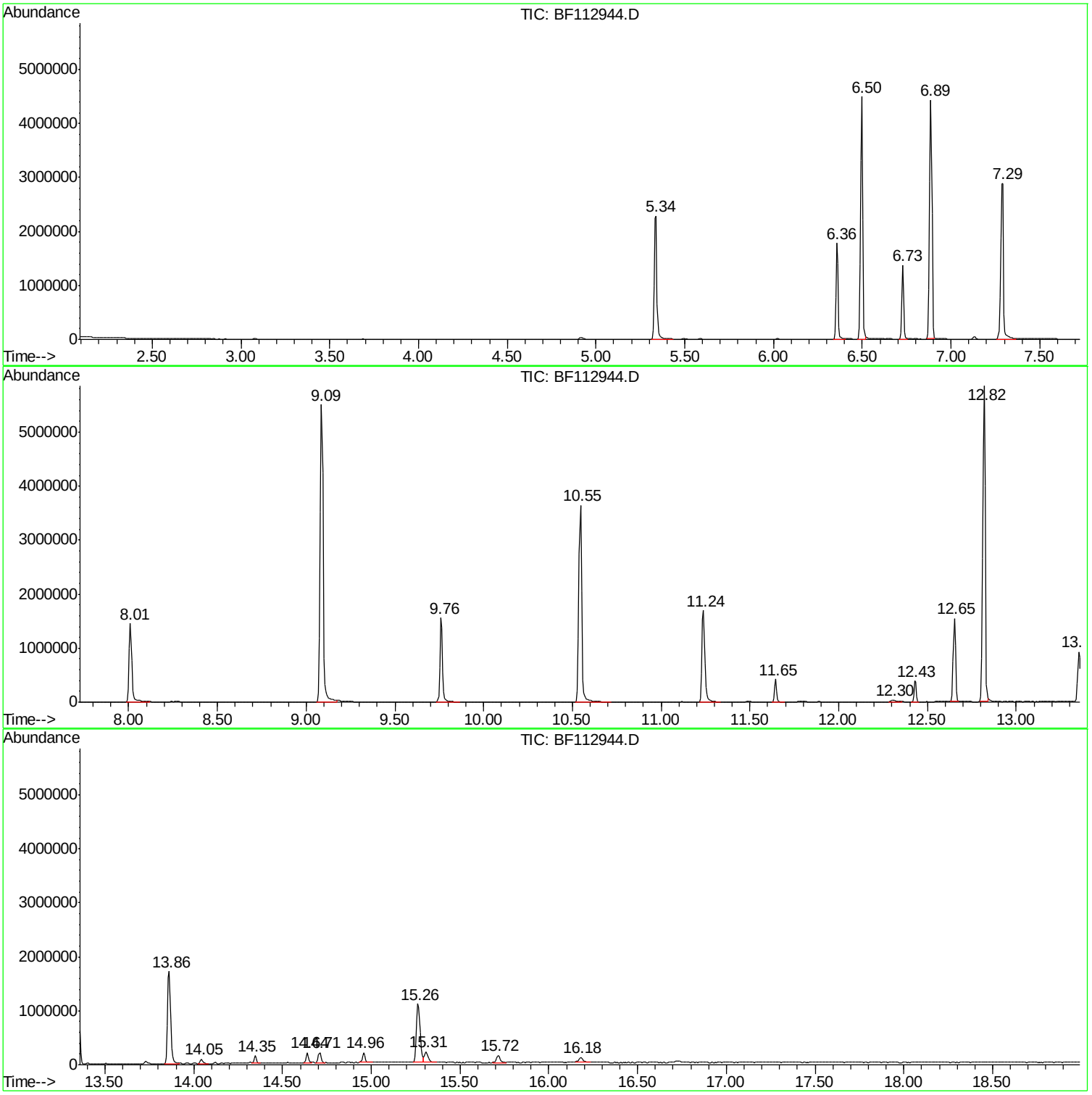
Instrument : BNA_F
ClientSampleId : FB-2019-03-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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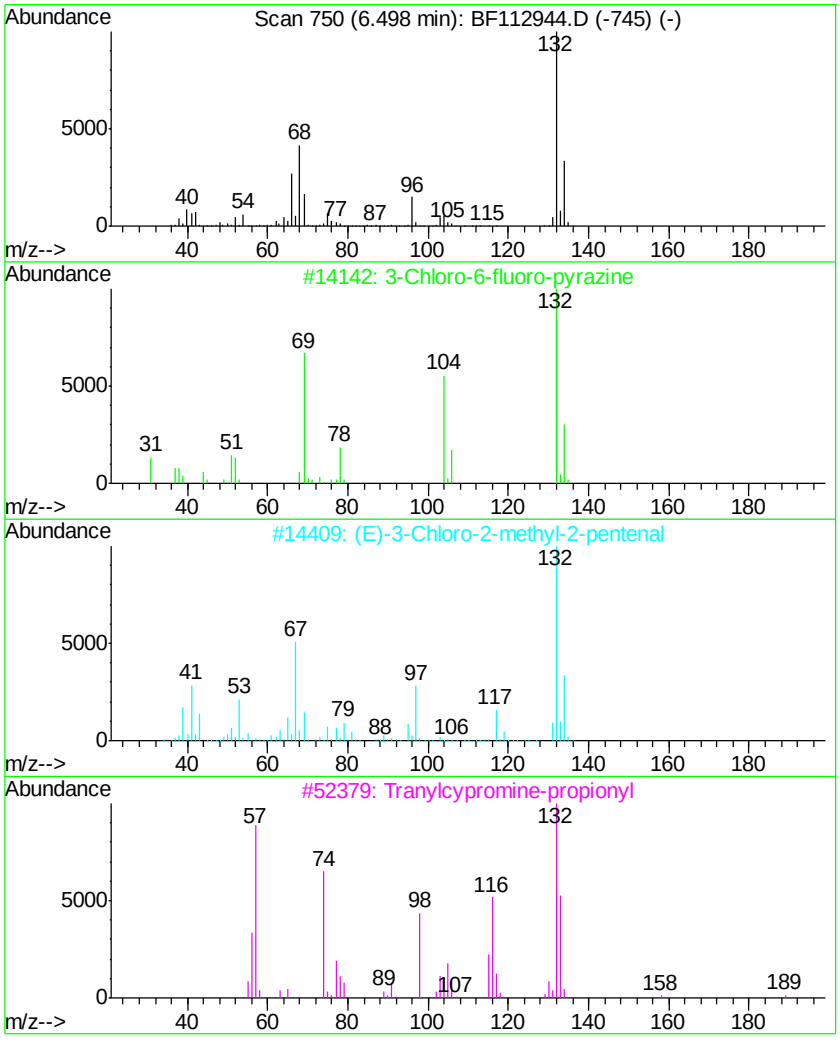
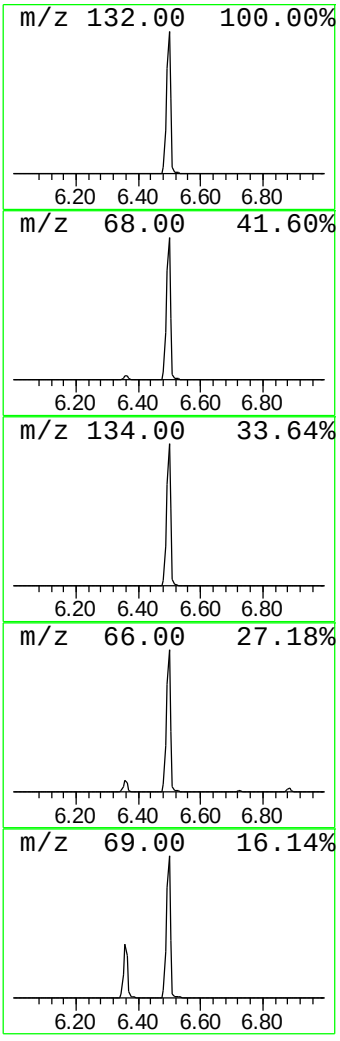
Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	73.96 ng	4194240	1,4-Dichlorobenzene-d4	6.73

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	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : FB-2019-03-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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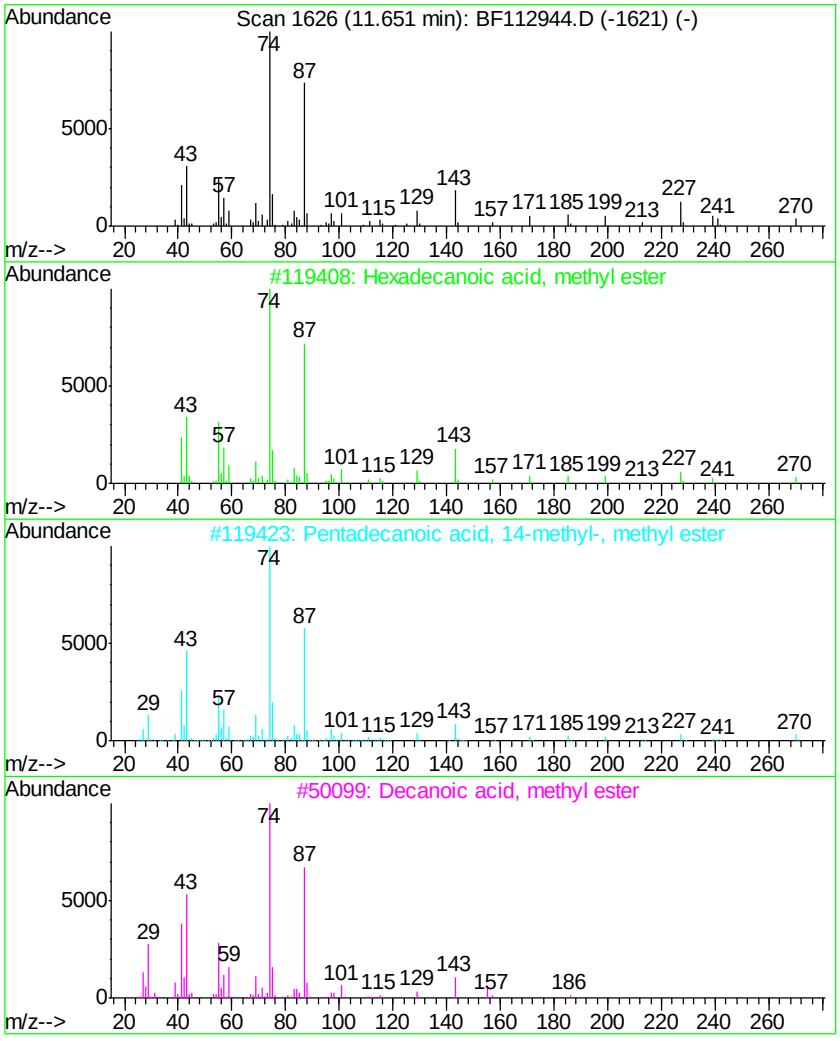
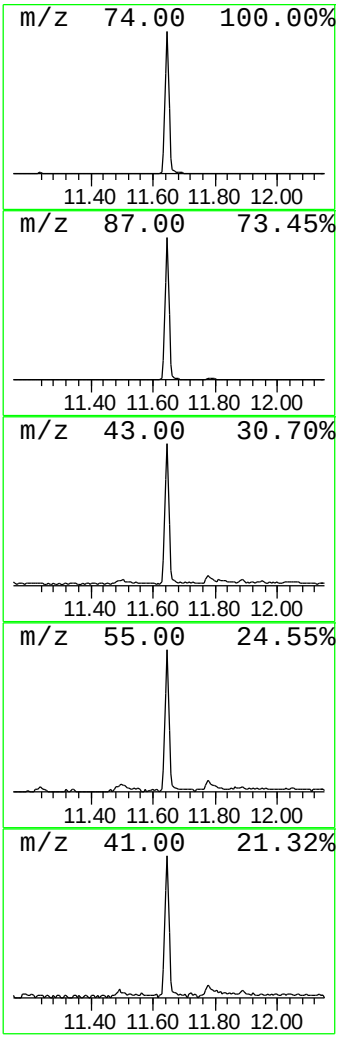
Peak Number 3 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	4.02 ng	364945	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
3	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	87
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86





Library Search Compound Report

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Operator : JU/SJ
Sample : K1783-08
Misc :
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Instrument : BNA_F
ClientSampleId : FB-2019-03-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

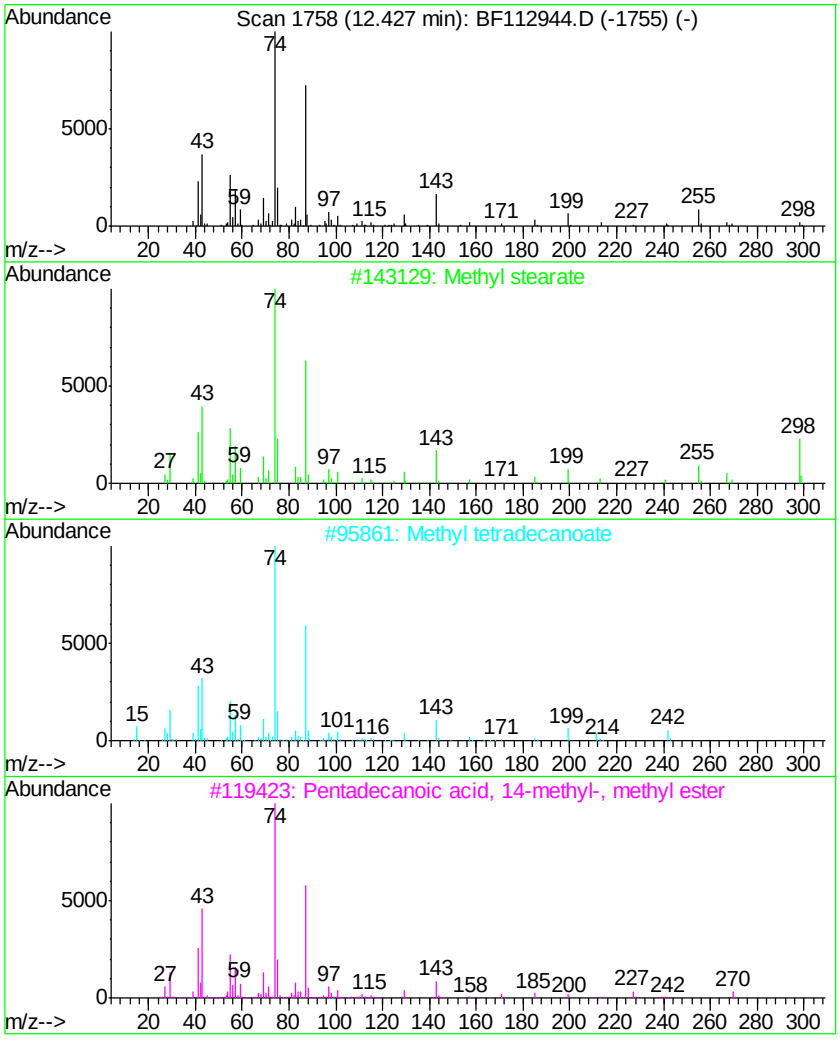
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

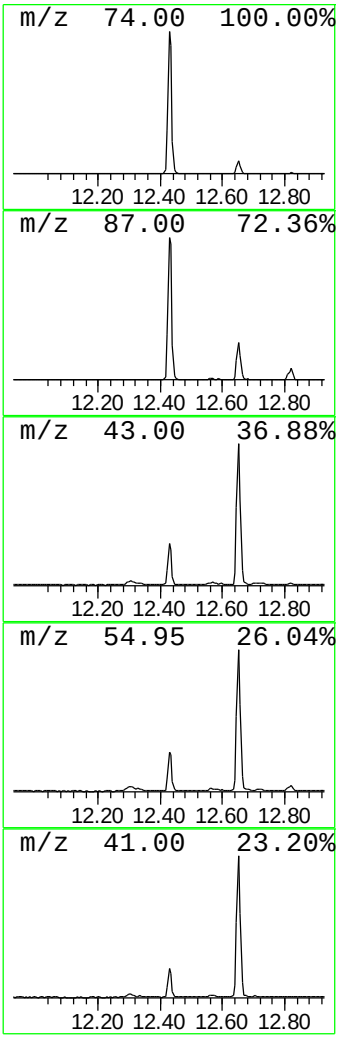
****

Peak Number 4 Methyl stearate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.43	3.80 ng	345241	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
4	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91





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Operator : JU/SJ
Sample : K1783-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-2019-03-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

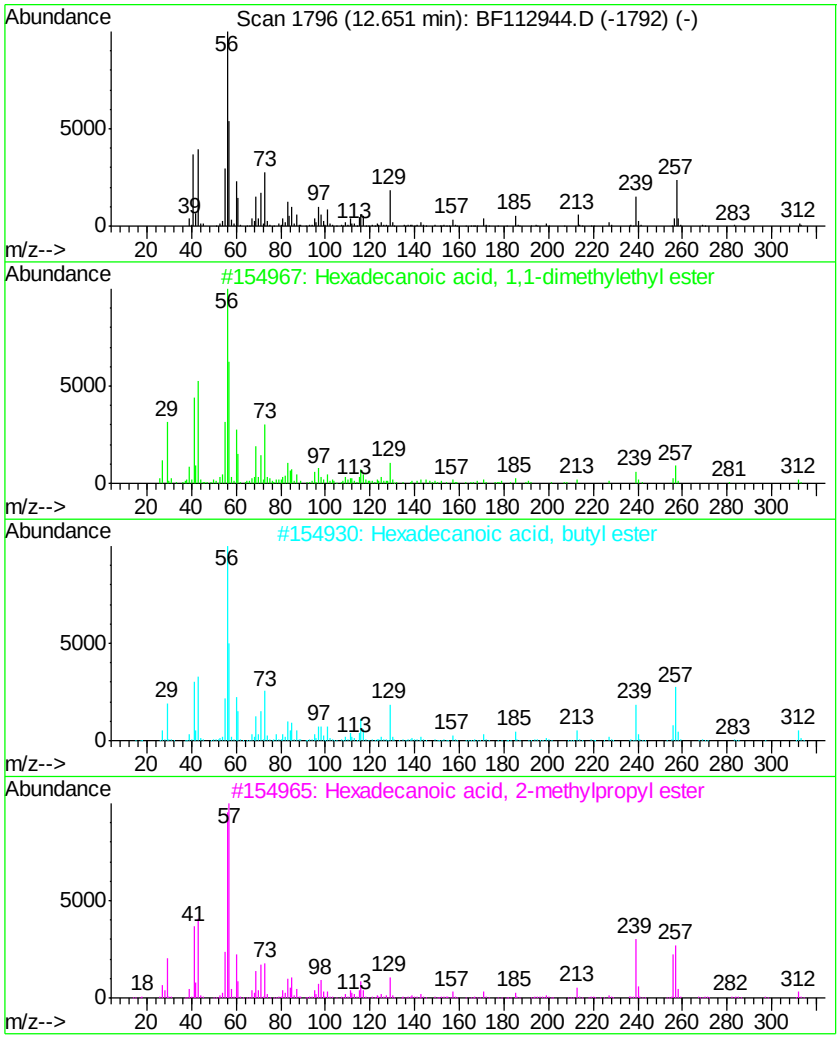
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

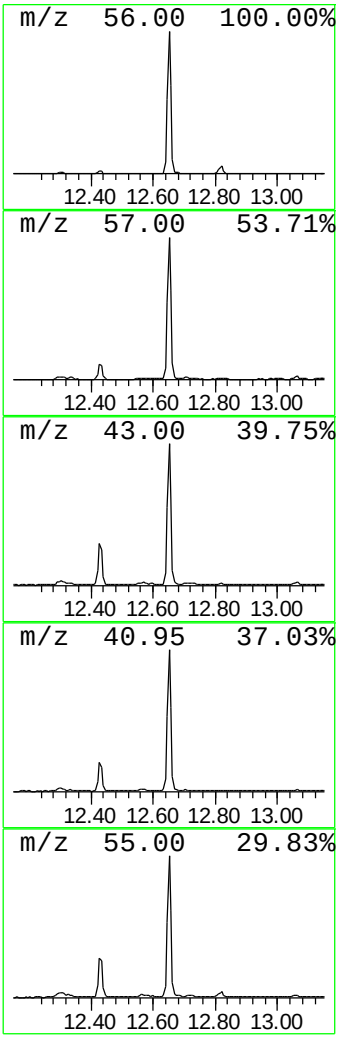
****

Peak Number 5 Hexadecanoic acid, 1,1-dime... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	13.26 ng	1290820	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	93
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30





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Operator : JU/SJ
Sample : K1783-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-2019-03-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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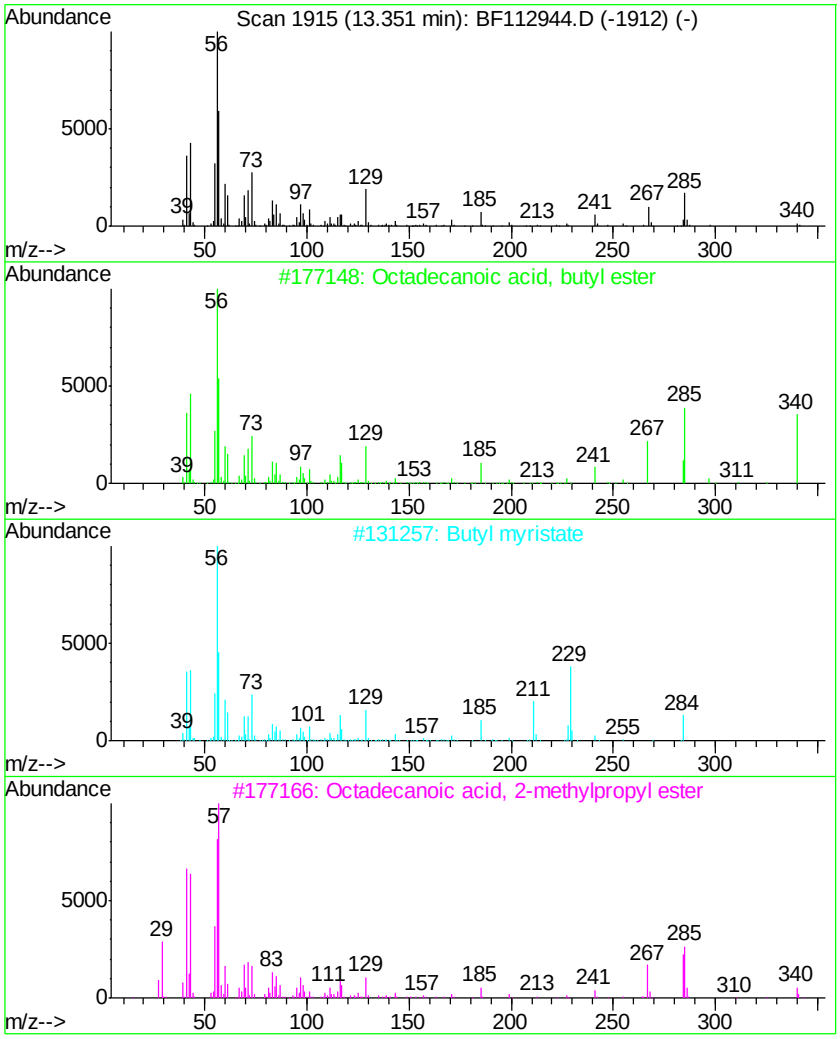
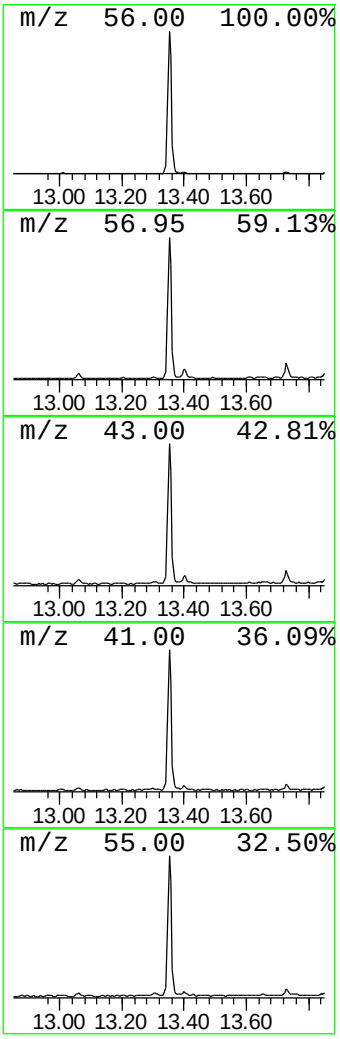
Peak Number 6 Octadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.35	8.49 ng	826396	Chrysene-d12	13.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2	Butyl myristate	284	C18H36O2	000110-36-1	80
3	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	46
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
5	2-Decene, 9-methyl-, (Z)-	154	C11H22	074630-24-3	32





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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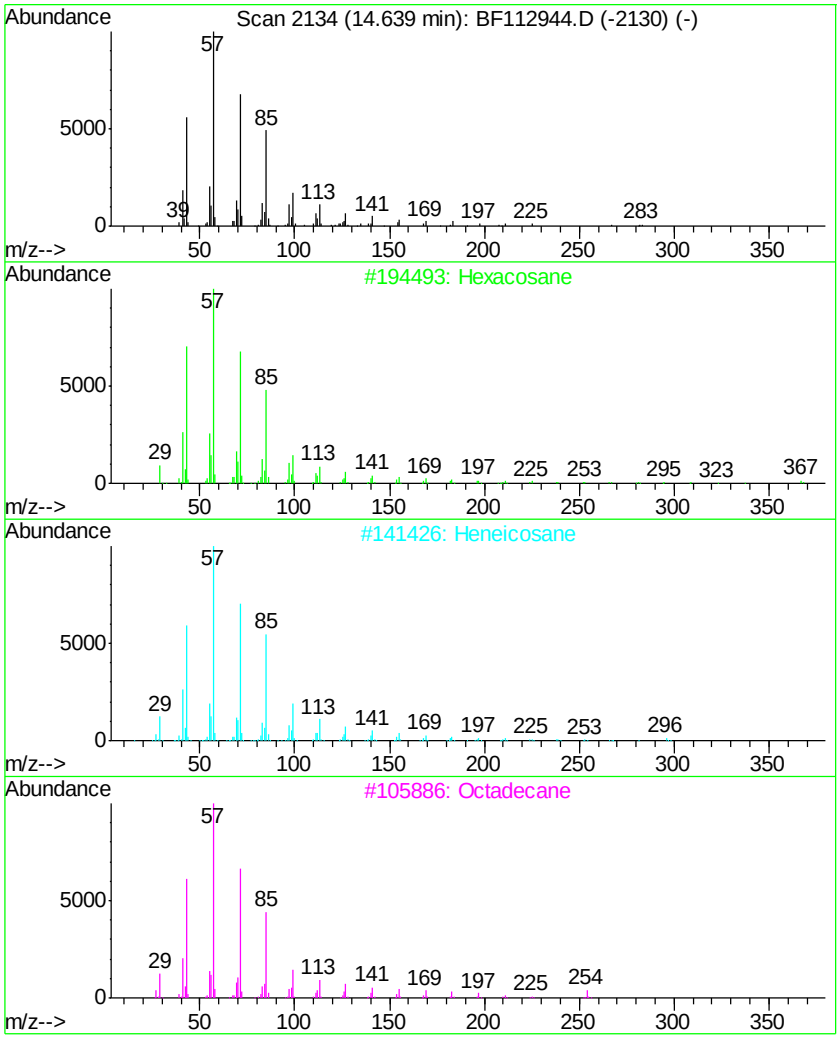
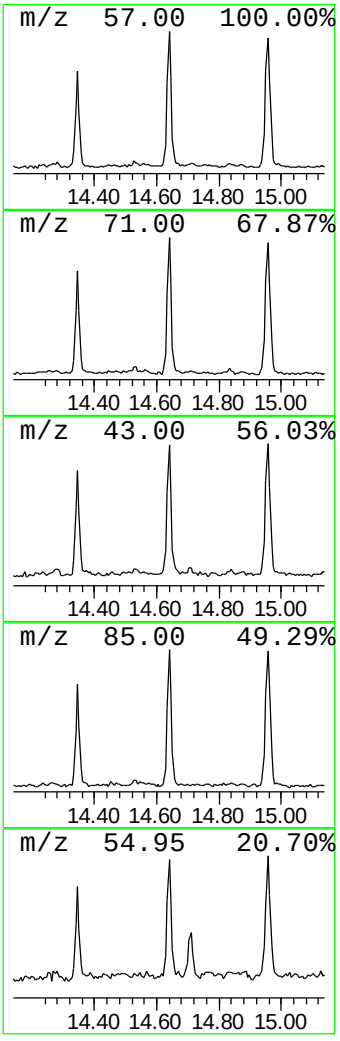
Peak Number 7 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.30 ng	177467	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Eicosane	282	C20H42	000112-95-8	87





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TIC Library : C:\DATABASE\NIST11.L
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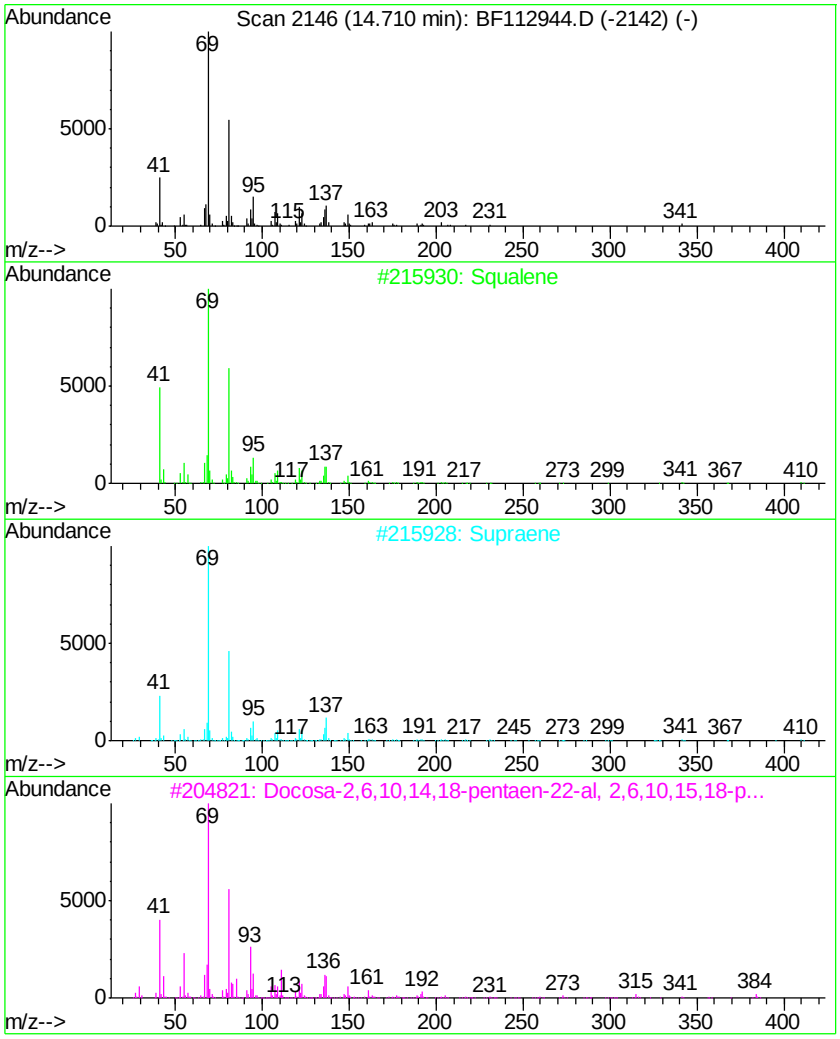
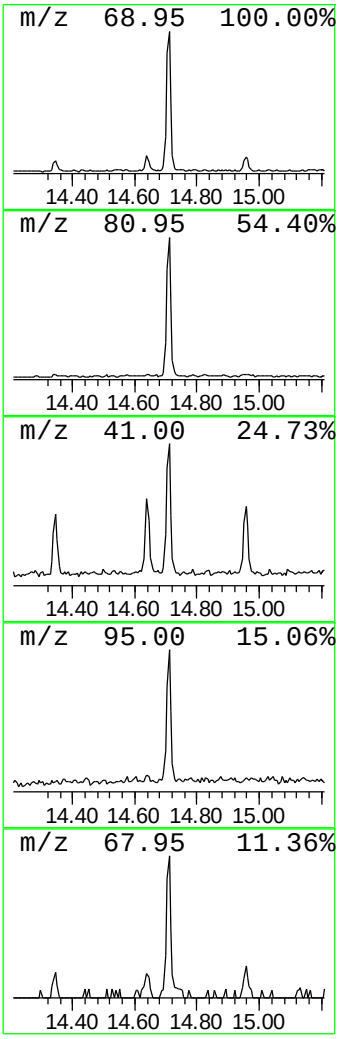
Peak Number 8 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	2.41 ng	186189	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	78
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





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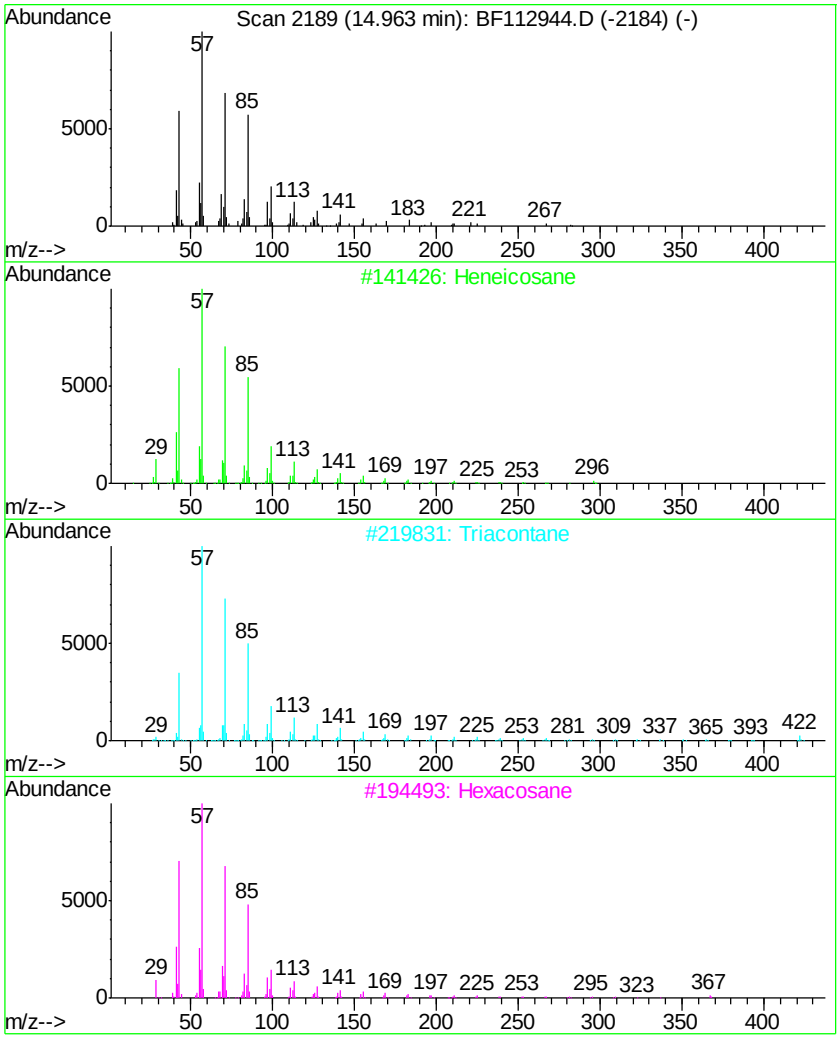
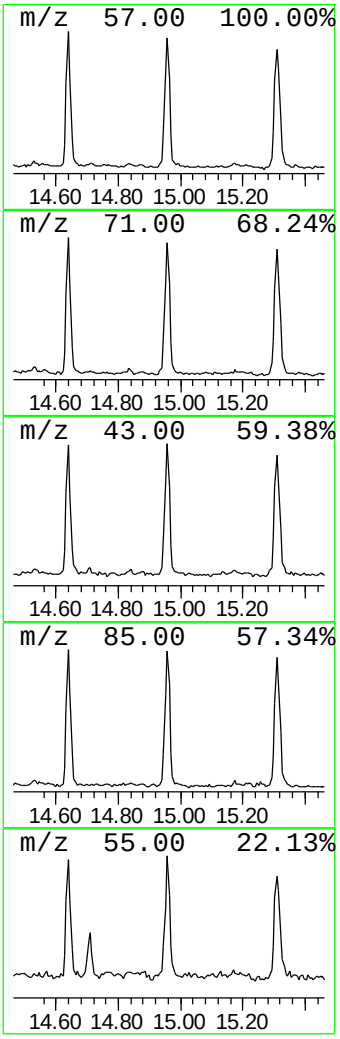
Peak Number 9 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.54 ng	195889	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-2019-03-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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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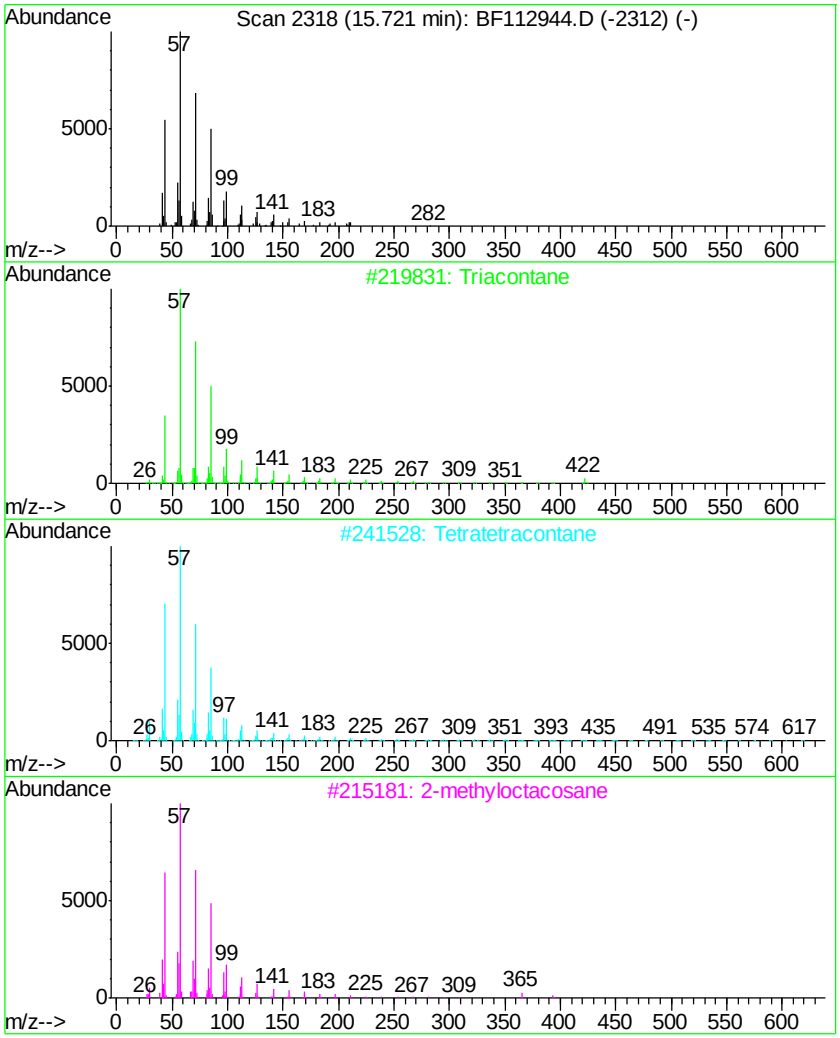
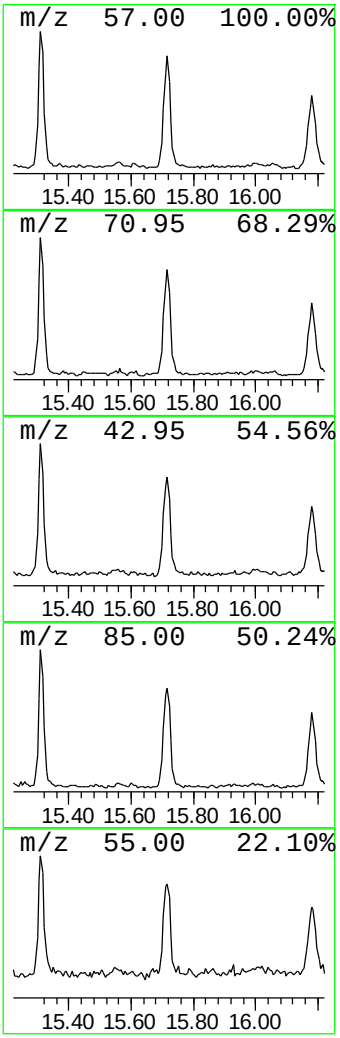
Peak Number 10 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	2.57 ng	198431	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Tetratetracontane	619	C44H90	007098-22-8	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
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Sample : K1783-08
Misc :
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Instrument : BNA_F
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TIC Integration Parameters: LSCINT.P

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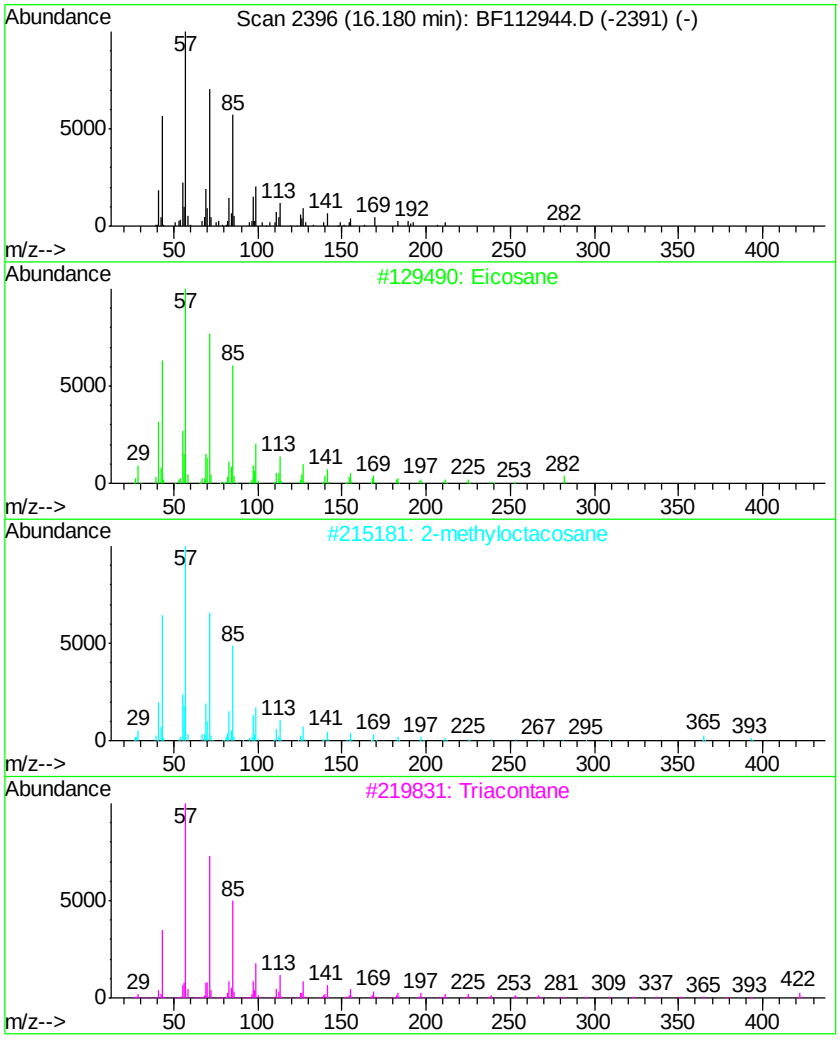
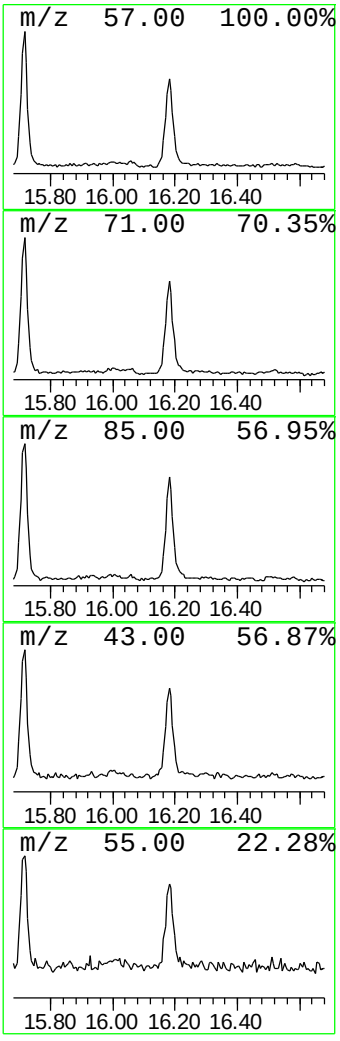
Peak Number 11 Eicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	2.06 ng	159143	Perylene-d12	15.26

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Heneicosane	296	C21H44	000629-94-7	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF030819\
Data File : BF112944.D
Acq On : 8 Mar 2019 15:11
Operator : JU/SJ
Sample : K1783-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FB-2019-03-05

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.50	6.50	74.0	ng	4194240	1	6.73	1134170	20.0
Hexadecanoic acid...	11.65	4.0	ng	364945	4	11.24	1816660	20.0
Methyl stearate	12.43	3.8	ng	345241	4	11.24	1816660	20.0
Hexadecanoic acid...	12.65	13.3	ng	1290820	5	13.86	1946330	20.0
Octadecanoic acid...	13.35	8.5	ng	826396	5	13.86	1946330	20.0
Hexacosane	14.64	2.3	ng	177467	6	15.26	1544660	20.0
Squalene	14.71	2.4	ng	186189	6	15.26	1544660	20.0
Heneicosane	14.96	2.5	ng	195889	6	15.26	1544660	20.0
Triacontane	15.72	2.6	ng	198431	6	15.26	1544660	20.0
Eicosane	16.18	2.1	ng	159143	6	15.26	1544660	20.0