LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112769.D
Acq On : 28 Feb 2019 19:02
Operator : JU/SJ
Sample : K1650-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-3(9-10)

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	5.363	551	557	560	rBV	5018768	5385017	90.38%	10.495%
2	6.381	724	730	733	rBV	4644120	5693916	95.56%	11.097%
3	6.516	748	753	756	rBV	5346753	5609762	94.15%	10.933%
4	6.745	788	792	795	rBV	1509574	1236729	20.76%	2.410%
5	6.904	814	819	822	rBV	4670546	4346906	72.95%	8.472%
6	7.304	881	887	890	rBV	3527427	3636580	61.03%	7.087%
7	8.022	1005	1009	1013	rBV	1633080	1525046	25.60%	2.972%
8	9.104	1187	1193	1196	rBV	6051532	5958343	100.00%	11.612%
9	9.492	1255	1259	1262	rBV	394864	363688	6.10%	0.709%
10	9.775	1302	1307	1314	rVB	1774984	1662260	27.90%	3.240%
11	10.557	1435	1440	1443	rBV	3716530	3542596	59.46%	6.904%
12	11.251	1554	1558	1561	rBV	1850090	1582556	26.56%	3.084%
13	11.786	1644	1649	1653	rBV	492437	473706	7.95%	0.923%
14	12.568	1777	1782	1791	rBV	246690	297851	5.00%	0.580%
15	12.710	1803	1806	1810	rBV	332714	309557	5.20%	0.603%
16	12.833	1823	1827	1830	rBV	4903475	4865661	81.66%	9.483%
17	13.733	1976	1980	1987	rBV3	238374	308127	5.17%	0.600%
18	13.874	2000	2004	2008	rBV	1511161	1262560	21.19%	2.461%
19	14.062	2032	2036	2041	rVB	141315	128700	2.16%	0.251%
20	14.362	2084	2087	2091	rBV	196274	184482	3.10%	0.360%
21	14.662	2135	2138	2143	rVB	308890	287759	4.83%	0.561%
22	14.980	2189	2192	2199	rVB	315220	338470	5.68%	0.660%
23	15.286	2239	2244	2248	rVV	1086257	1250795	20.99%	2.438%
24	15.339	2249	2253	2260	rVB	321631	400632	6.72%	0.781%
25	15.745	2318	2322	2327	rBV	251331	368285	6.18%	0.718%
26	16.221	2399	2403	2408	rVB	185130	291949	4.90%	0.569%

Sum of corrected areas: 51311933

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Misc :
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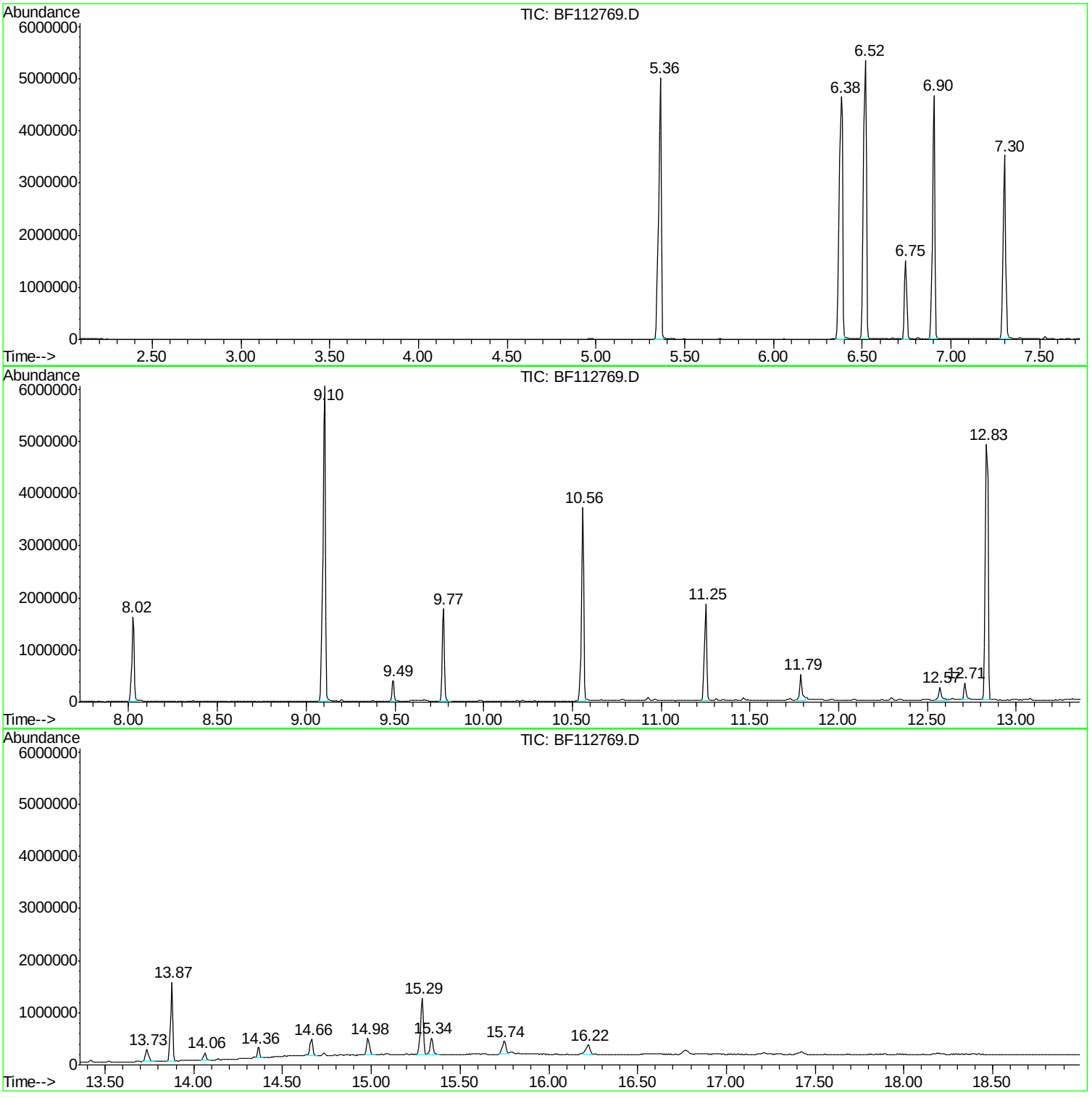
Instrument :
BNA_F
ClientSampleId :
B-3(9-10)

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



Library Search Compound Report

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Data File : BF112769.D
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Instrument : BNA_F
ClientSampleId : B-3(9-10)

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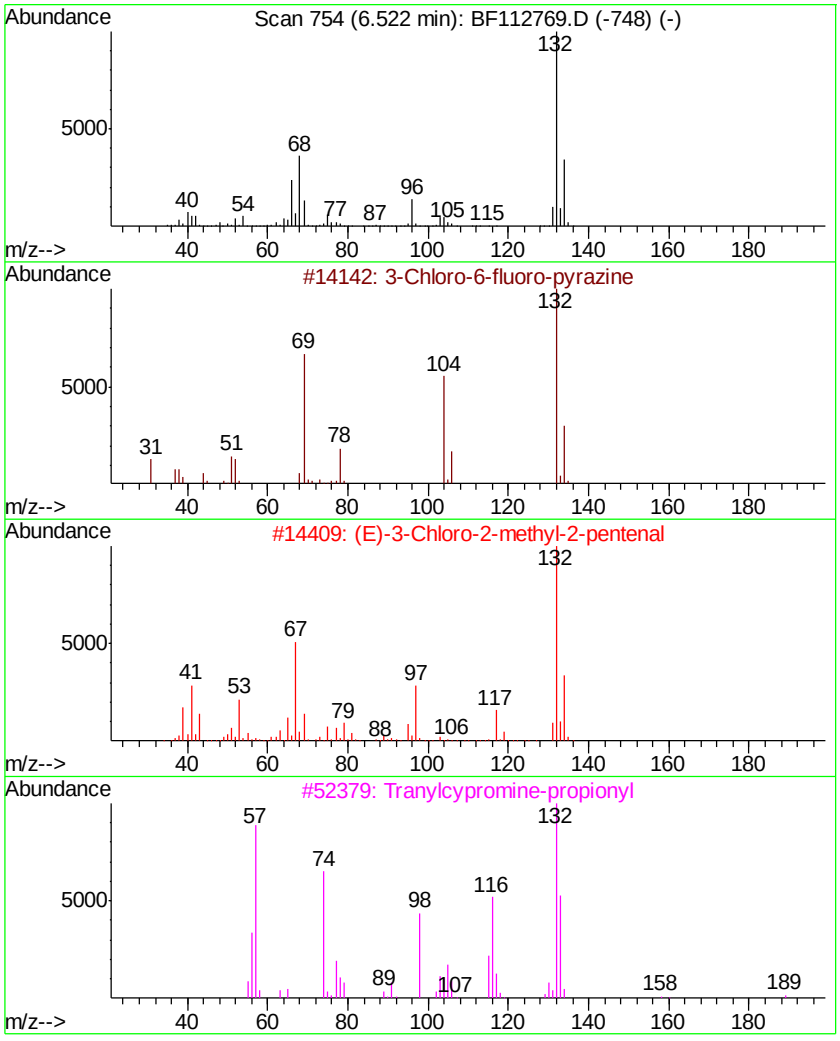
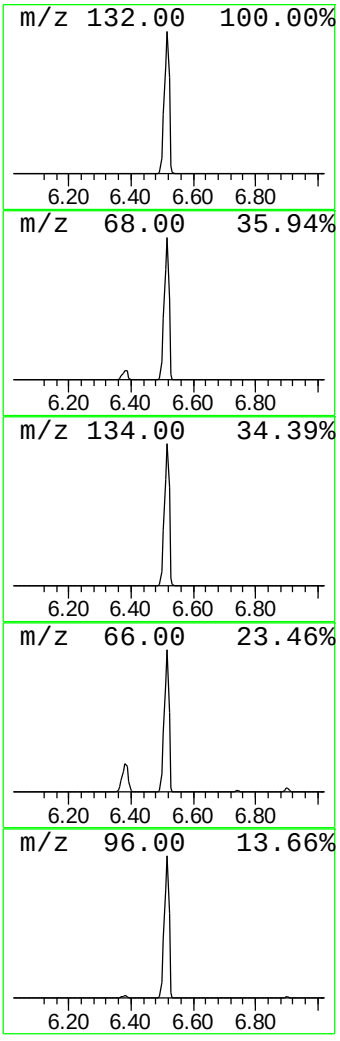
Peak Number 1 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	90.72 ng	5609760	1,4-Dichlorobenzene-d4	6.75

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	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : B-3(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
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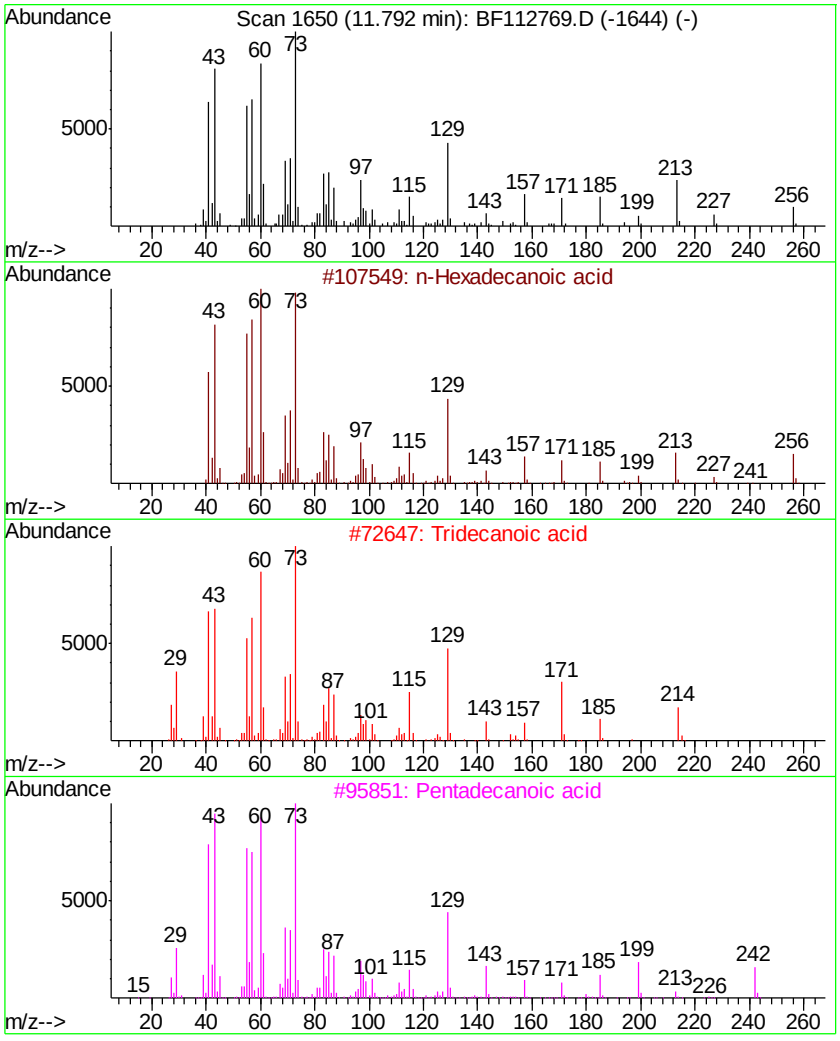
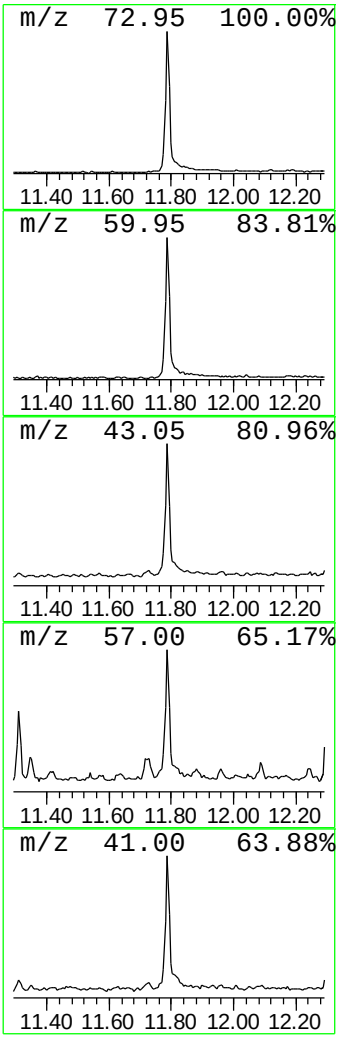
Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	5.99 ng	473706	Phenanthrene-d10	11.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Dodecanoic acid	200	C12H24O2	000143-07-7	83





Library Search Compound Report

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Data File : BF112769.D
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Operator : JU/SJ
Sample : K1650-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-3(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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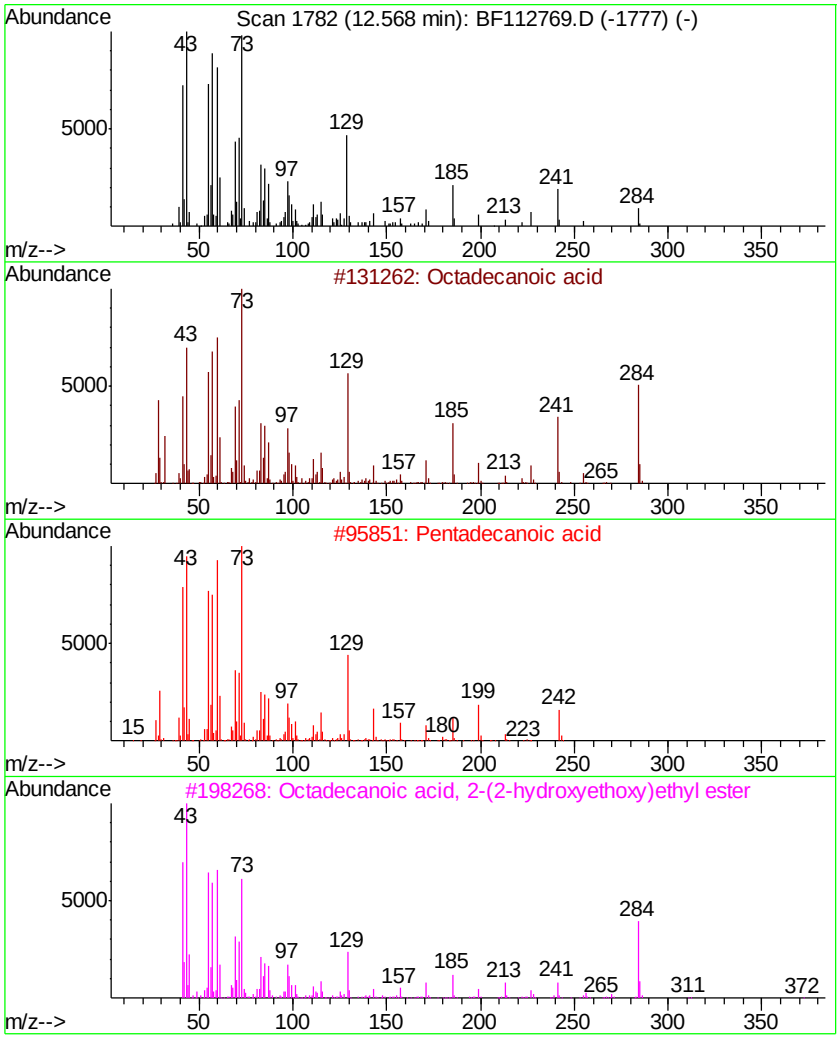
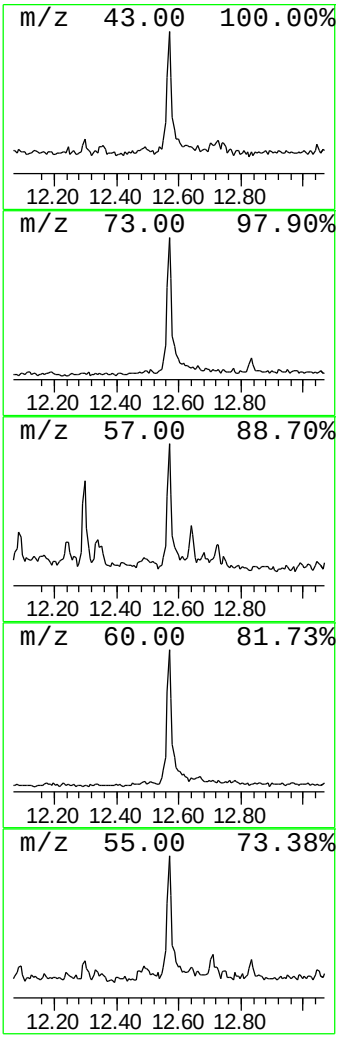
Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	4.72 ng	297851	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Operator : JU/SJ
Sample : K1650-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-3(9-10)

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

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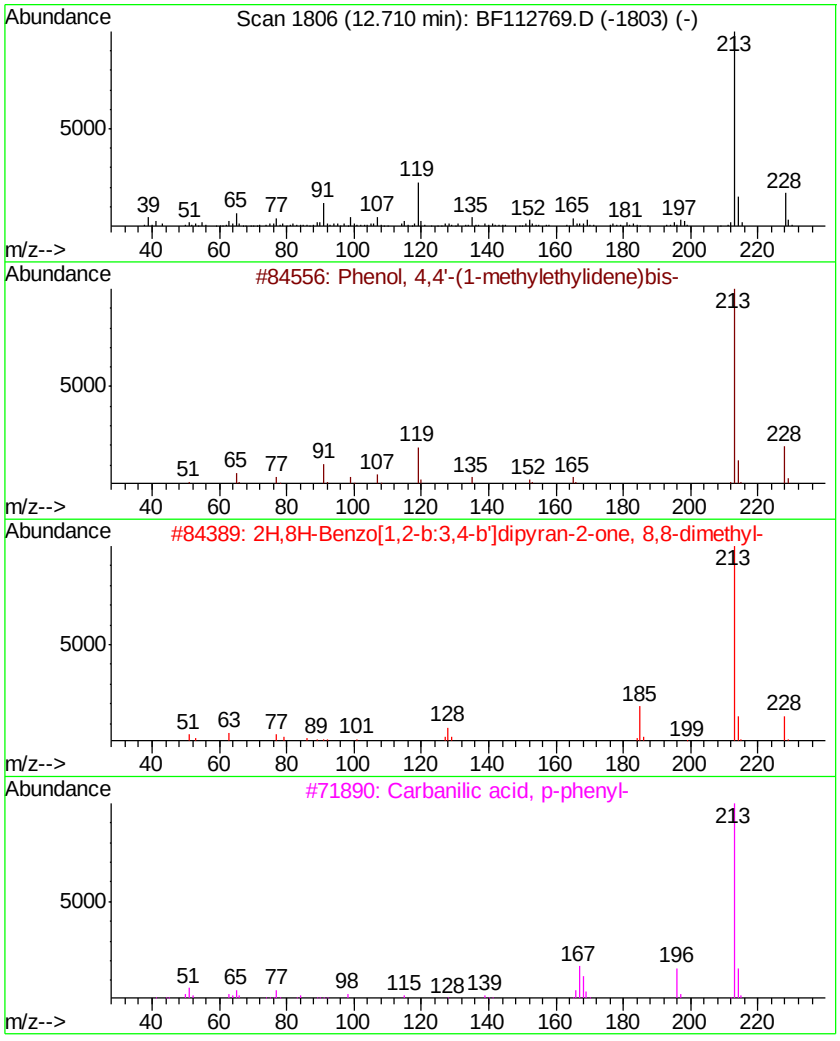
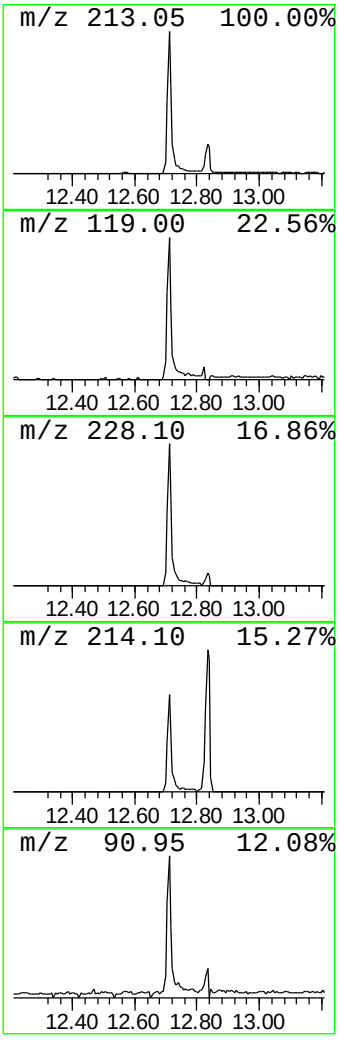
Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	4.90 ng	309557	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	53
3	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	49
4	Phenol, 2,4'-isopropylidenedi-	228	C15H16O2	000837-08-1	43
5	2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	42





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Operator : JU/SJ
Sample : K1650-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-3(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
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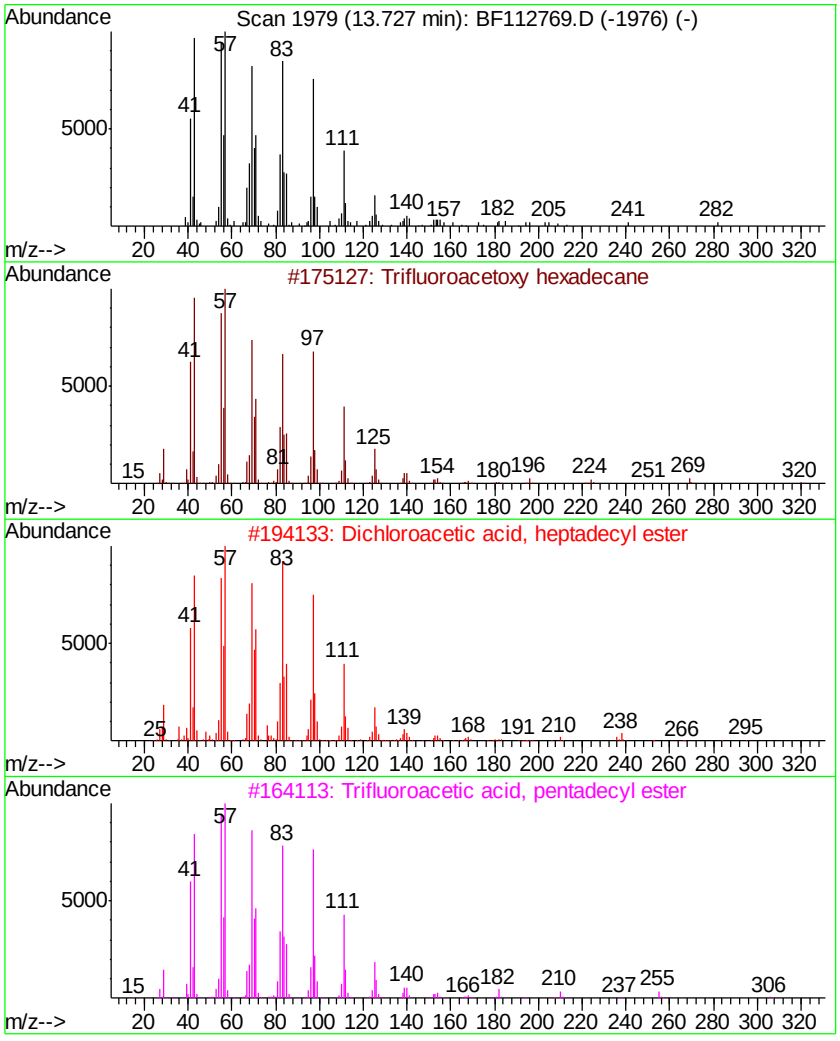
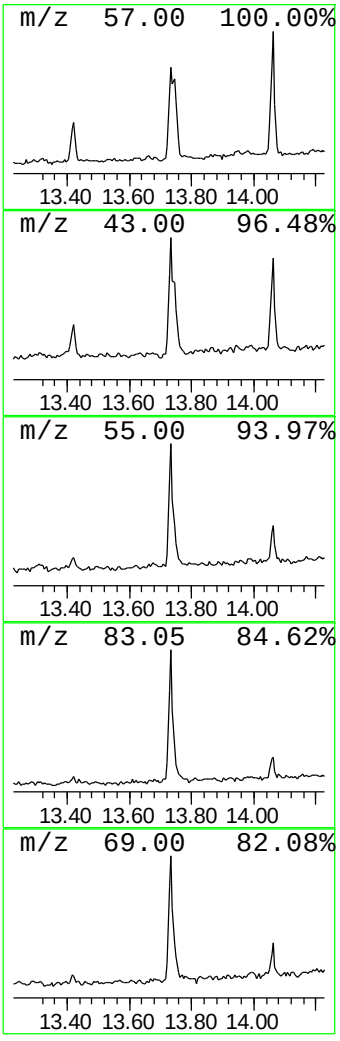
Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.88 ng	308127	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : B-3(9-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
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TIC Library : C:\DATABASE\NIST11.L
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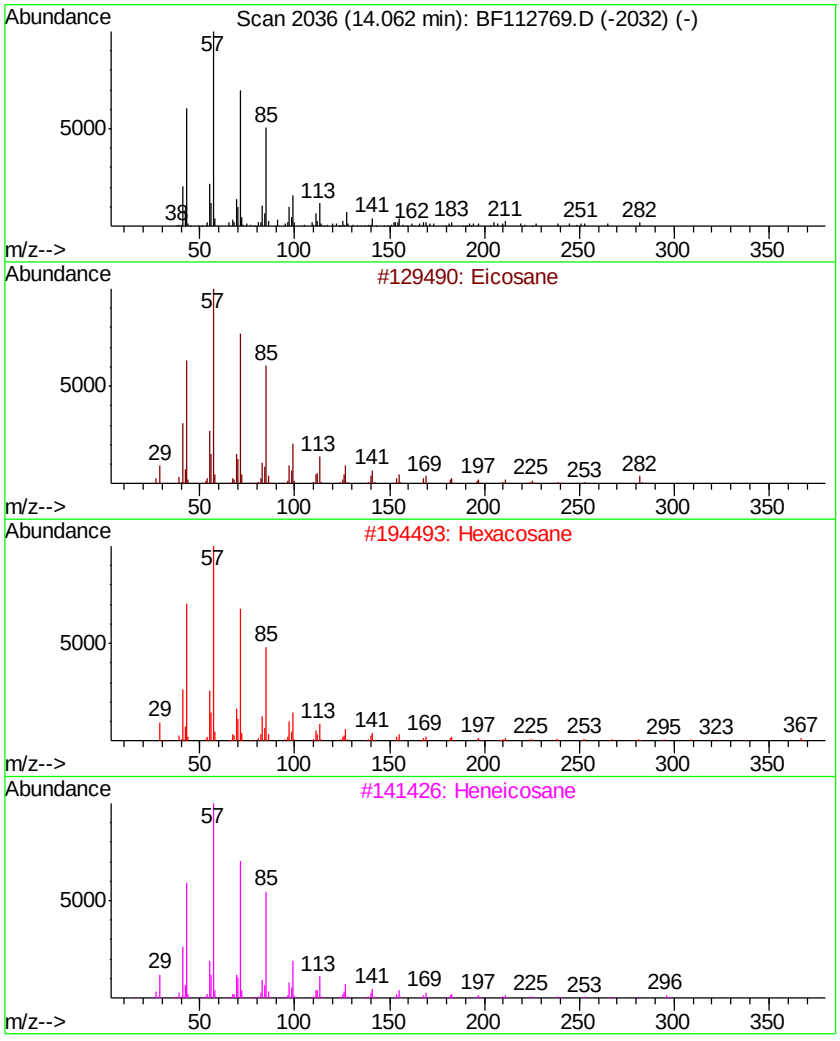
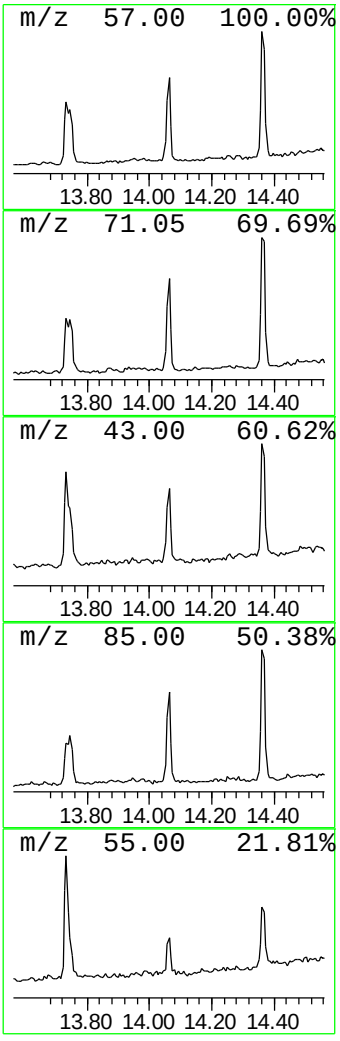
Peak Number 7 Eicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	2.04 ng	128700	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Hexacosane	366	C26H54	000630-01-3	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octacosane	394	C28H58	000630-02-4	87
5	Nonadecane	268	C19H40	000629-92-5	87





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Instrument : BNA_F
ClientSampleId : B-3(9-10)

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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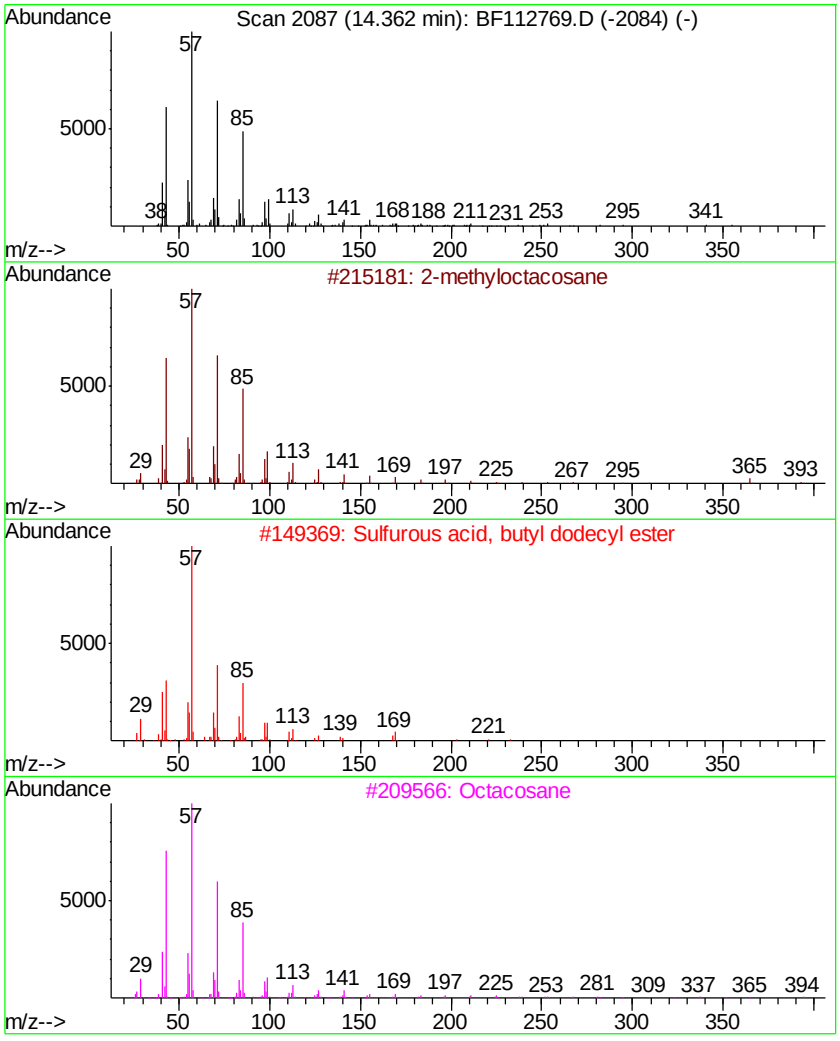
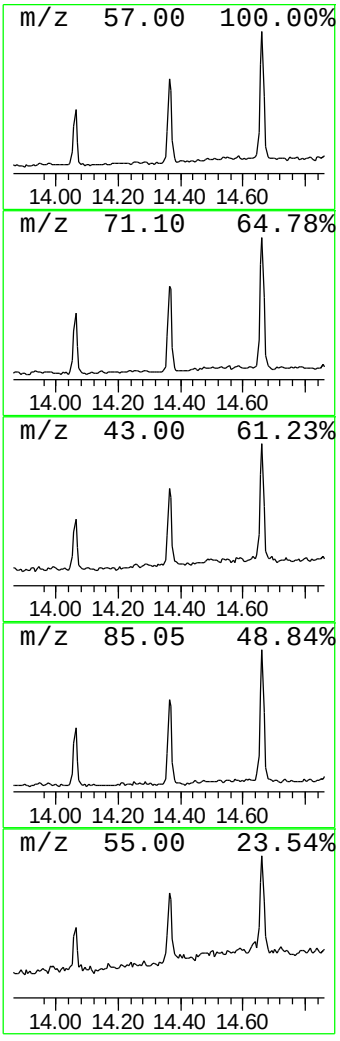
Peak Number 8 2-methyloctacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	2.92 ng	184482	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	91
3	Octacosane	394	C28H58	000630-02-4	87
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
5	Octadecane	254	C18H38	000593-45-3	80





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Instrument : BNA_F
ClientSampleId : B-3(9-10)

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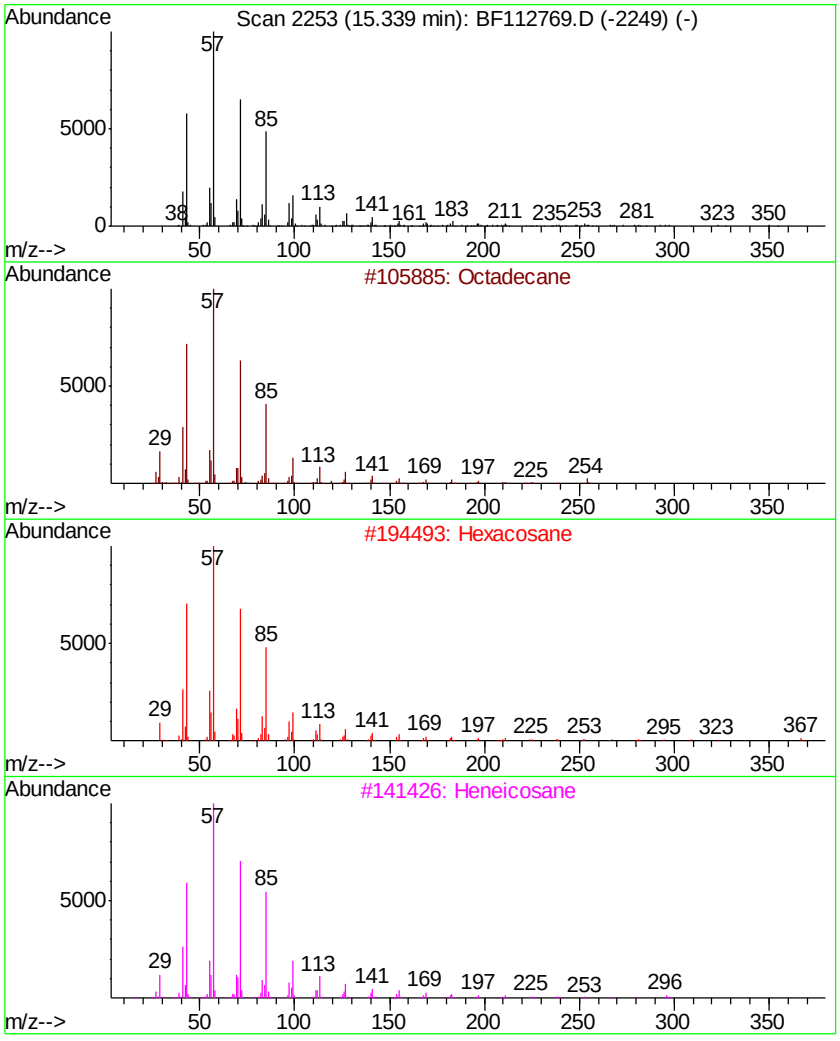
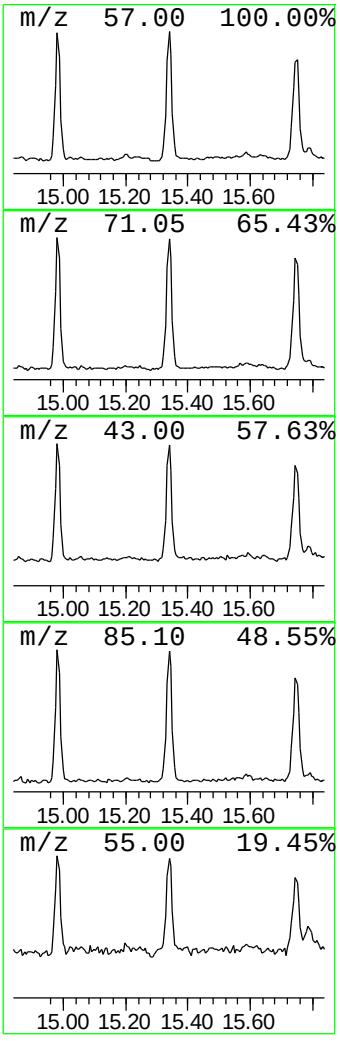
****

Peak Number 11 Octadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.34	6.41 ng	400632	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	95
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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Instrument : BNA_F
ClientSampleId : B-3(9-10)

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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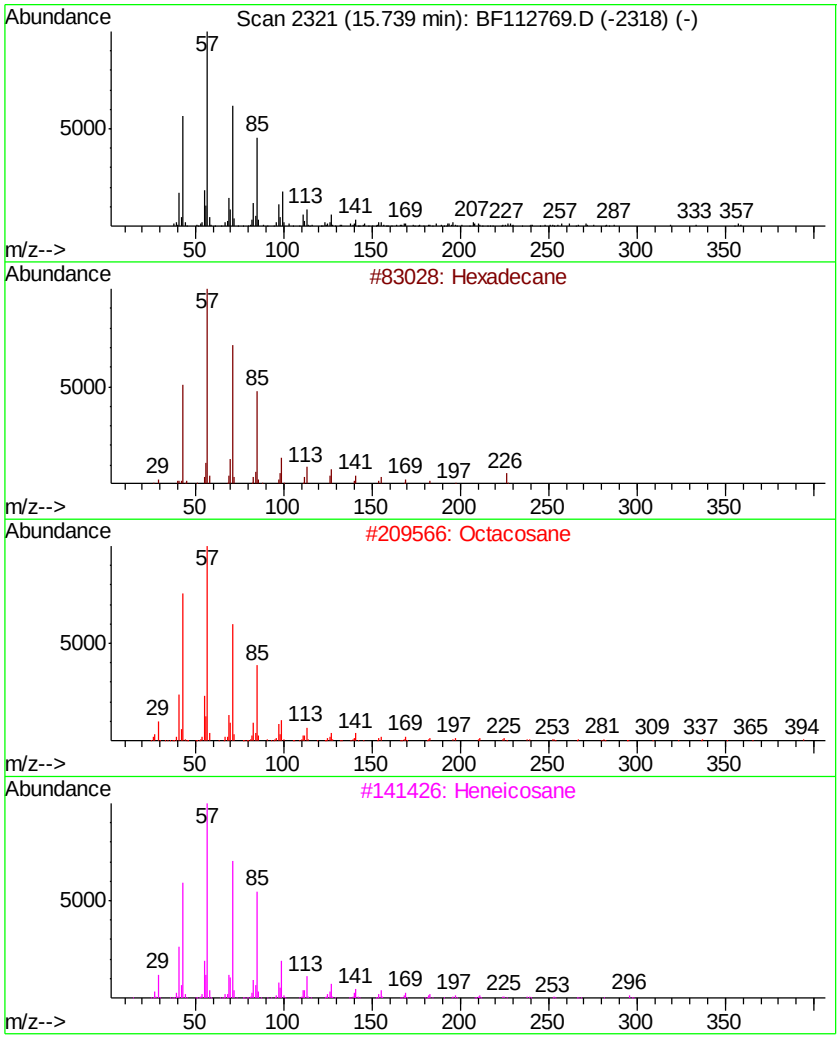
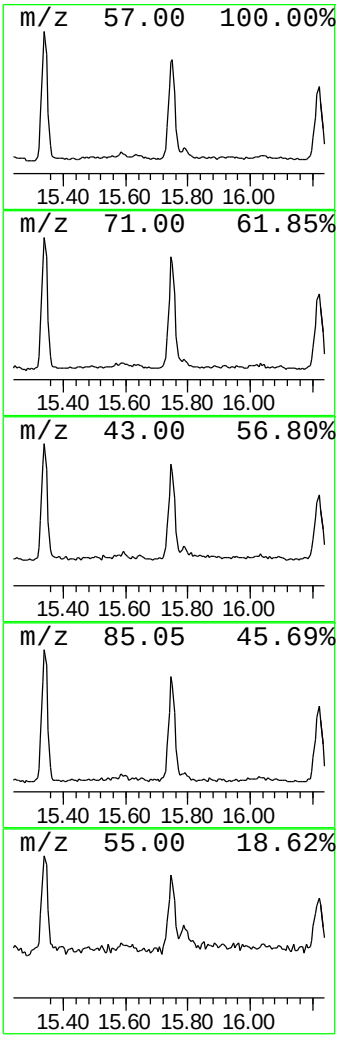
Peak Number 12 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	5.89 ng	368285	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	93
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Tetracosane	338	C24H50	000646-31-1	90





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Instrument : BNA_F
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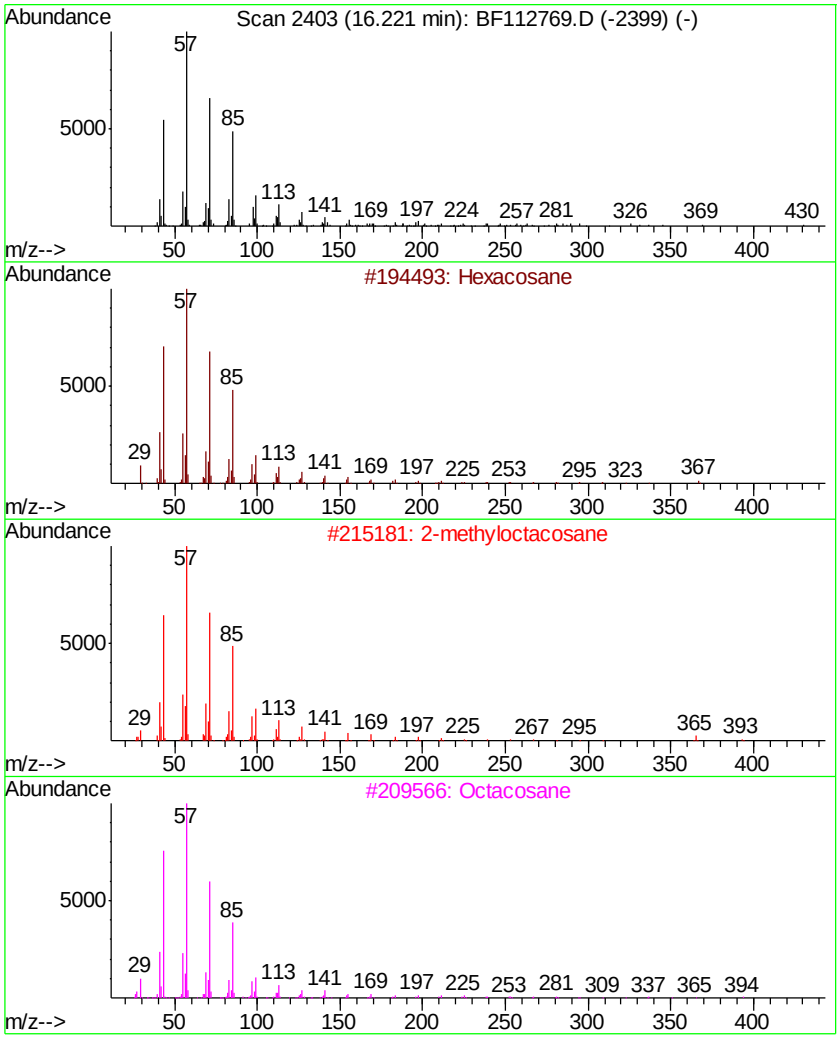
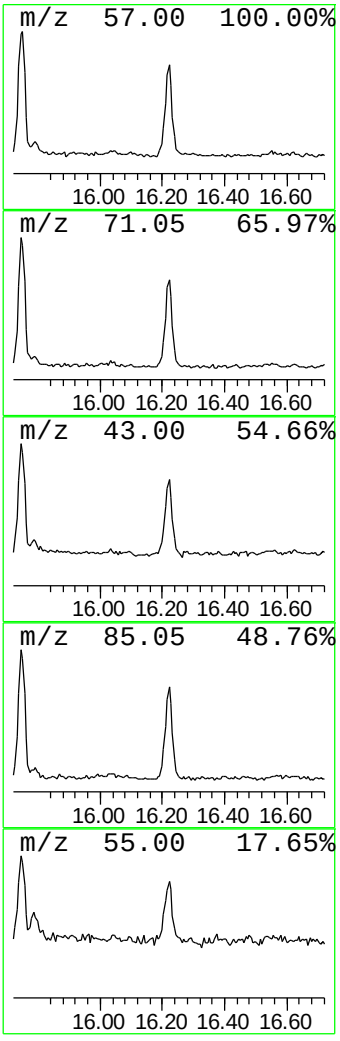
Peak Number 13 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.22	4.67 ng	291949	Perylene-d12	15.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	90
3	Octacosane	394	C28H58	000630-02-4	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Eicosane	282	C20H42	000112-95-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
Data File : BF112769.D
Acq On : 28 Feb 2019 19:02
Operator : JU/SJ
Sample : K1650-07
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-3(9-10)

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
unknown6.52	6.52	90.7	ng	5609760	1	6.75	1236730	20.0
n-Hexadecanoic acid	11.79	6.0	ng	473706	4	11.25	1582560	20.0
Octadecanoic acid	12.57	4.7	ng	297851	5	13.87	1262560	20.0
Phenol, 4,4'-(1-m...	12.71	4.9	ng	309557	5	13.87	1262560	20.0
Trifluoroacetoxy ...	13.73	4.9	ng	308127	5	13.87	1262560	20.0
Eicosane	14.06	2.0	ng	128700	5	13.87	1262560	20.0
2-methyloctacosane	14.36	2.9	ng	184482	5	13.87	1262560	20.0
Octadecane	15.34	6.4	ng	400632	6	15.29	1250800	20.0
Hexadecane	15.74	5.9	ng	368285	6	15.29	1250800	20.0
Hexacosane	16.22	4.7	ng	291949	6	15.29	1250800	20.0