LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112773.D
Acq On : 28 Feb 2019 20:51
Operator : JU/SJ
Sample : K1650-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6(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	4.951	478	487	494	rVB	34489	52252	1.05%	0.122%
2	5.357	550	556	559	rBV	4250776	4343364	87.01%	10.103%
3	6.381	724	730	733	rBV	4116176	4583138	91.81%	10.661%
4	6.510	747	752	756	rBV	4310161	4551970	91.19%	10.589%
5	6.745	788	792	795	rBV	1201607	1100527	22.05%	2.560%
6	6.898	814	818	822	rBV	3832749	3522452	70.56%	8.194%
7	7.304	881	887	890	rBV	2737377	2939468	58.88%	6.838%
8	8.022	1005	1009	1013	rBV	1587015	1378168	27.61%	3.206%
9	9.098	1188	1192	1196	rBV	5308351	4991901	100.00%	11.612%
10	9.375	1235	1239	1244	rBV	71984	67523	1.35%	0.157%
11	9.486	1255	1258	1265	rBV	343819	309185	6.19%	0.719%
12	9.775	1302	1307	1315	rVB	1573214	1563038	31.31%	3.636%
13	10.557	1435	1440	1443	rBV	3339625	3089035	61.88%	7.186%
14	11.251	1554	1558	1561	rBV	1616552	1519694	30.44%	3.535%
15	11.786	1643	1649	1662	rBV2	422740	461556	9.25%	1.074%
16	12.569	1778	1782	1790	rBV	169492	194240	3.89%	0.452%
17	12.710	1802	1806	1810	rBV	137522	146667	2.94%	0.341%
18	12.833	1822	1827	1830	rBV	4621267	4322361	86.59%	10.054%
19	13.733	1976	1980	1987	rBV2	180521	239238	4.79%	0.557%
20	13.874	2000	2004	2007	rBV	1294222	1162972	23.30%	2.705%
21	14.063	2031	2036	2041	rBV	115353	122100	2.45%	0.284%
22	14.363	2084	2087	2091	rBV	184585	162182	3.25%	0.377%
23	14.657	2134	2137	2142	rVB	210123	217901	4.37%	0.507%
24	14.980	2188	2192	2197	rBV	249404	260796	5.22%	0.607%
25	15.280	2238	2243	2248	rVB	950581	1185796	23.75%	2.758%
26	15.339	2248	2253	2257	rBV	206550	262281	5.25%	0.610%
27	15.745	2317	2322	2326	rBV	169103	239767	4.80%	0.558%

Sum of corrected areas: 42989572

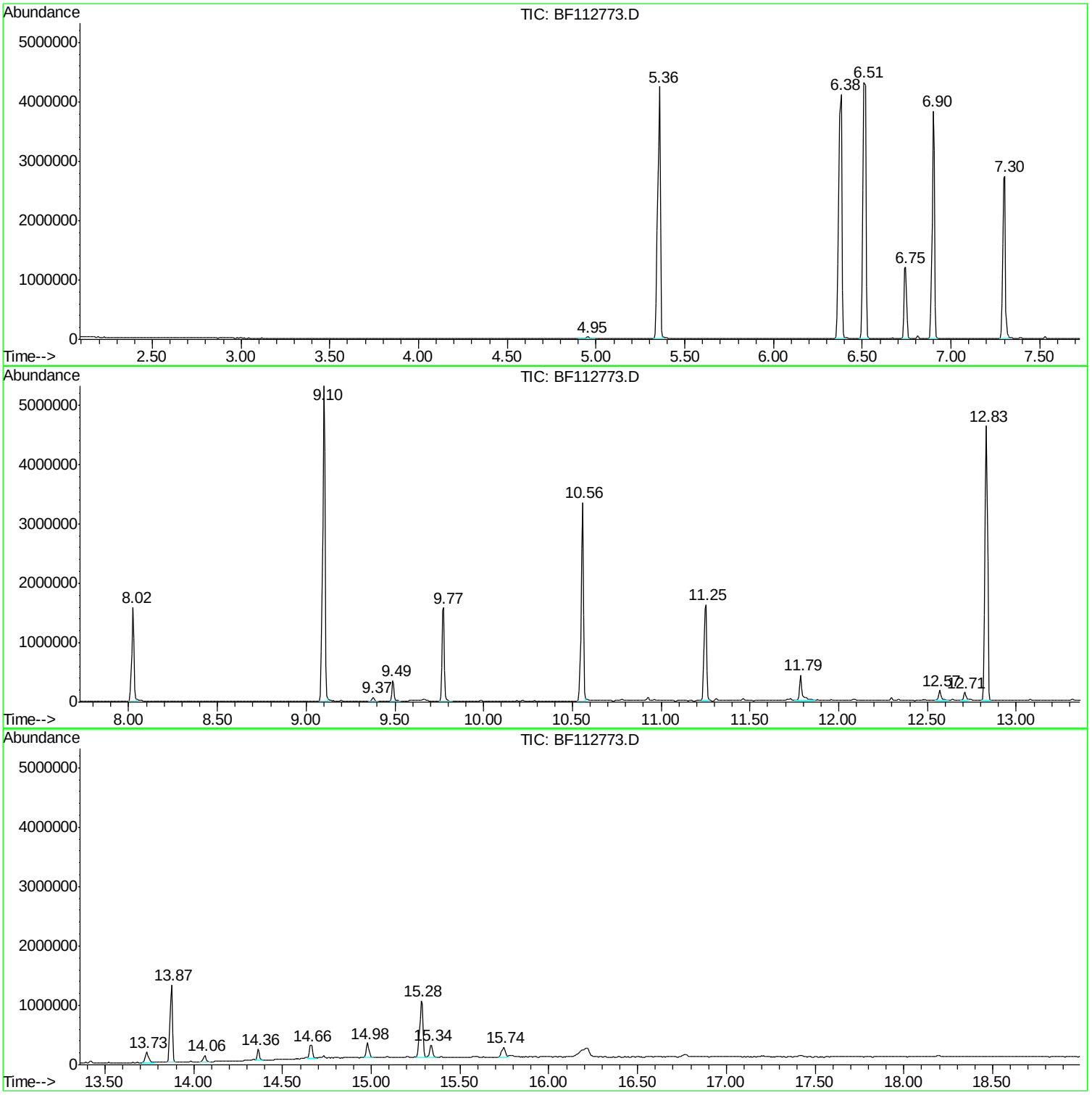
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112773.D
Acq On : 28 Feb 2019 20:51
Operator : JU/SJ
Sample : K1650-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-6(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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Misc :
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Instrument : BNA_F
ClientSampleId : B-6(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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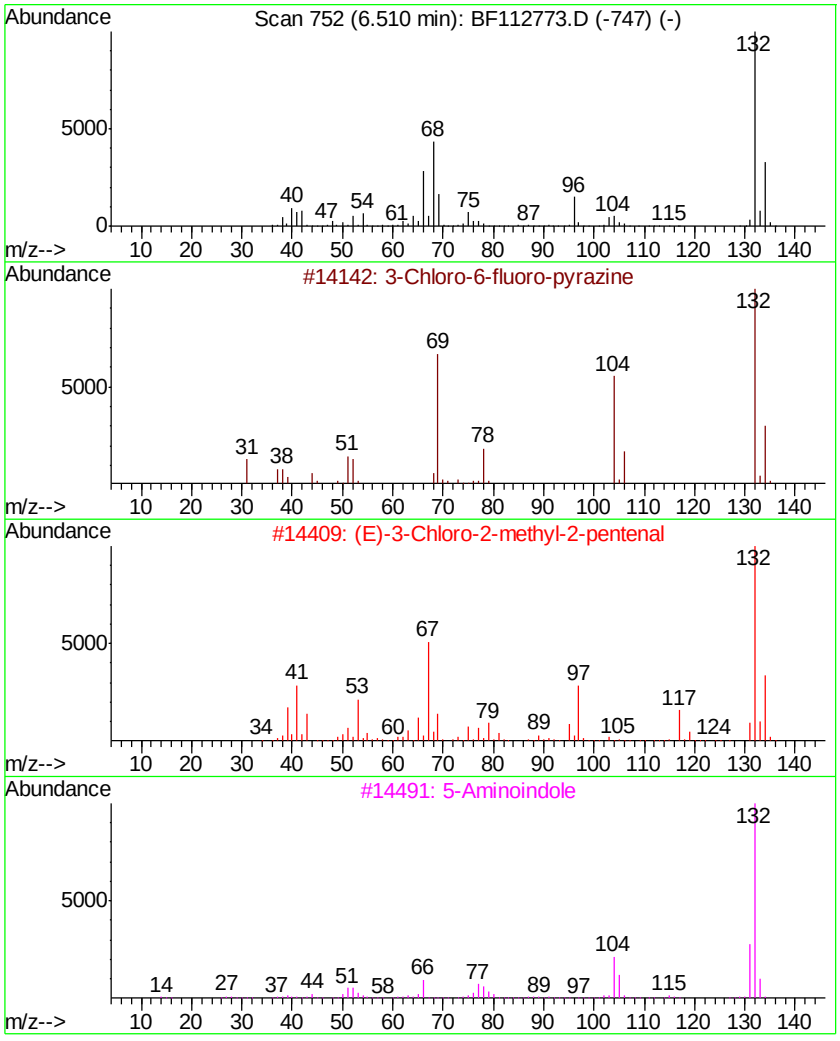
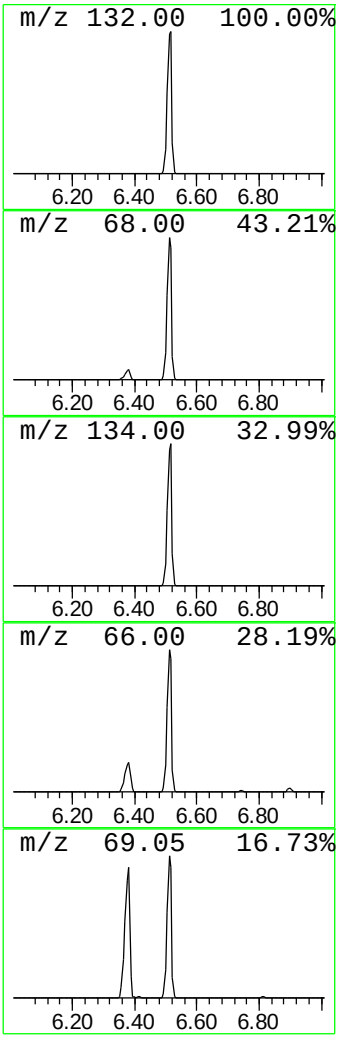
Peak Number 1 unknown6.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	82.72 ng	4551970	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	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Operator : JU/SJ
Sample : K1650-13
Misc :
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Instrument : BNA_F
ClientSampleId : B-6(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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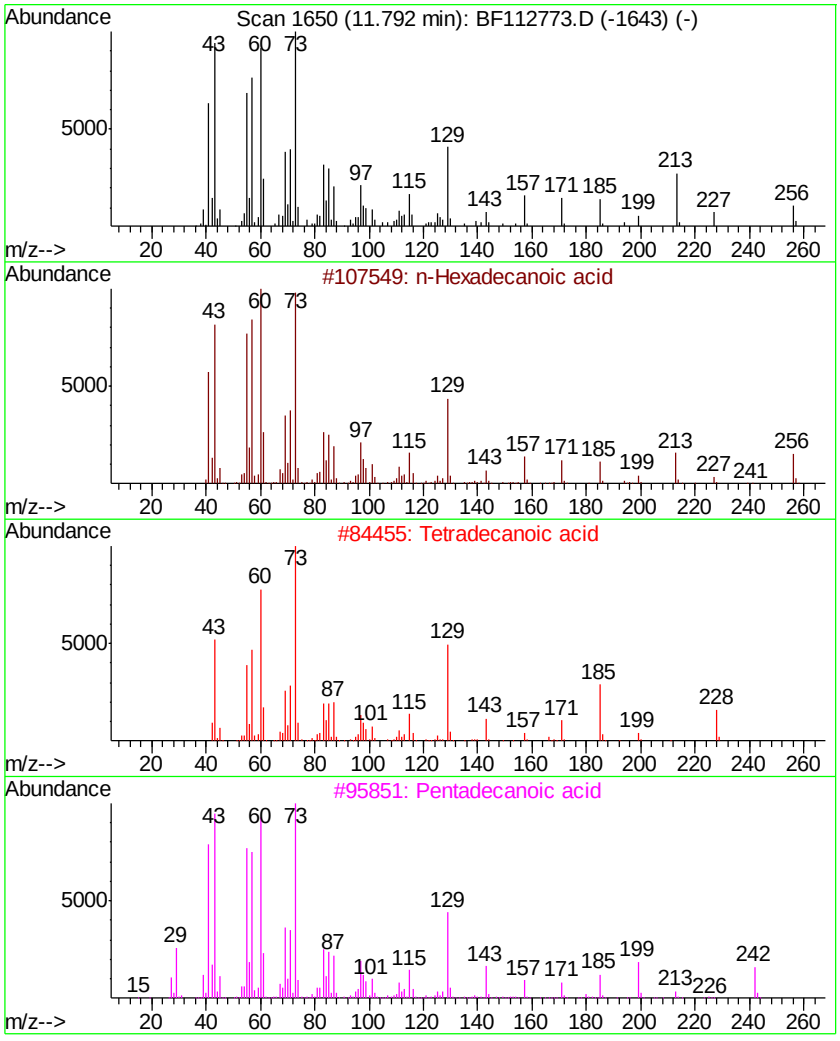
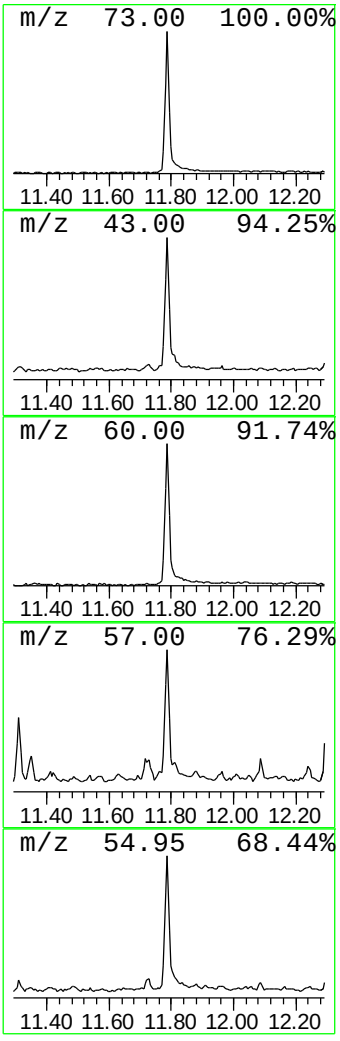
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	6.07 ng	461556	Phenanthrene-d10	11.25

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	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Nonanoic acid	158	C9H18O2	000112-05-0	43





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Data File : BF112773.D
Acq On : 28 Feb 2019 20:51
Operator : JU/SJ
Sample : K1650-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6(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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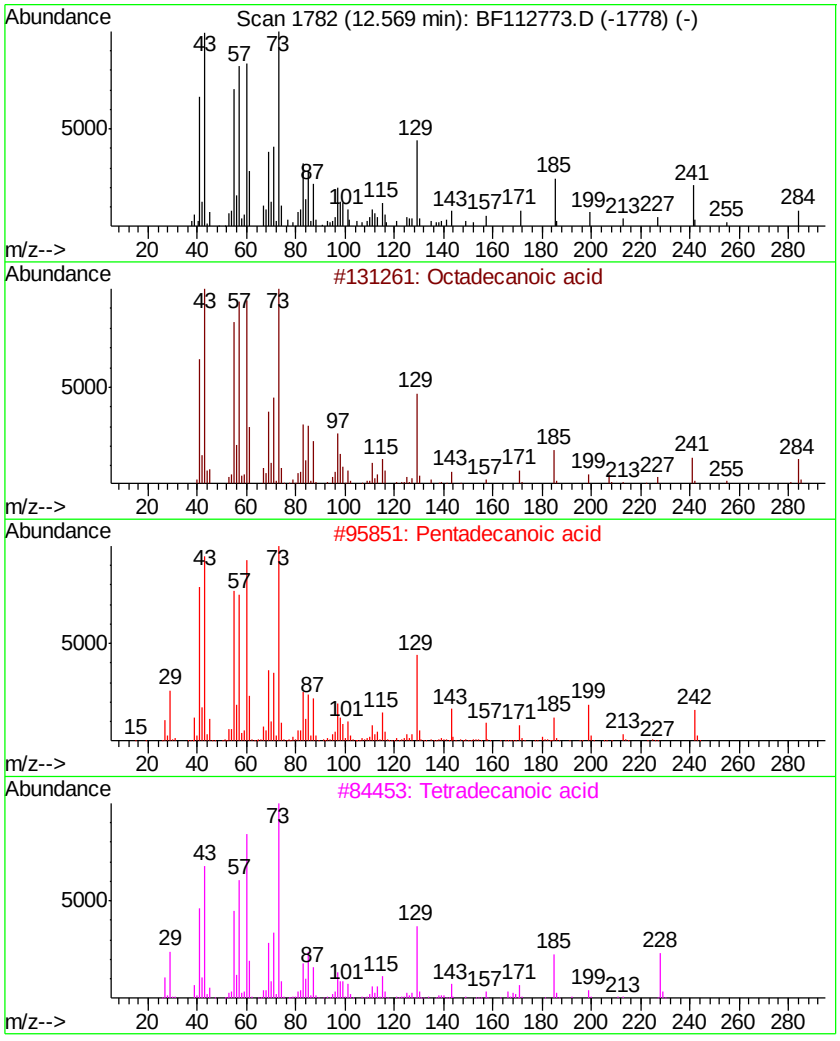
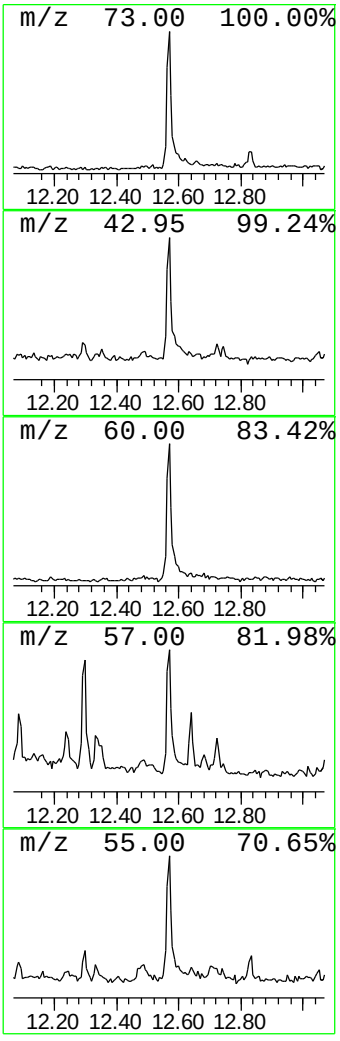
Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	3.34 ng	194240	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	52
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112773.D
Acq On : 28 Feb 2019 20:51
Operator : JU/SJ
Sample : K1650-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6(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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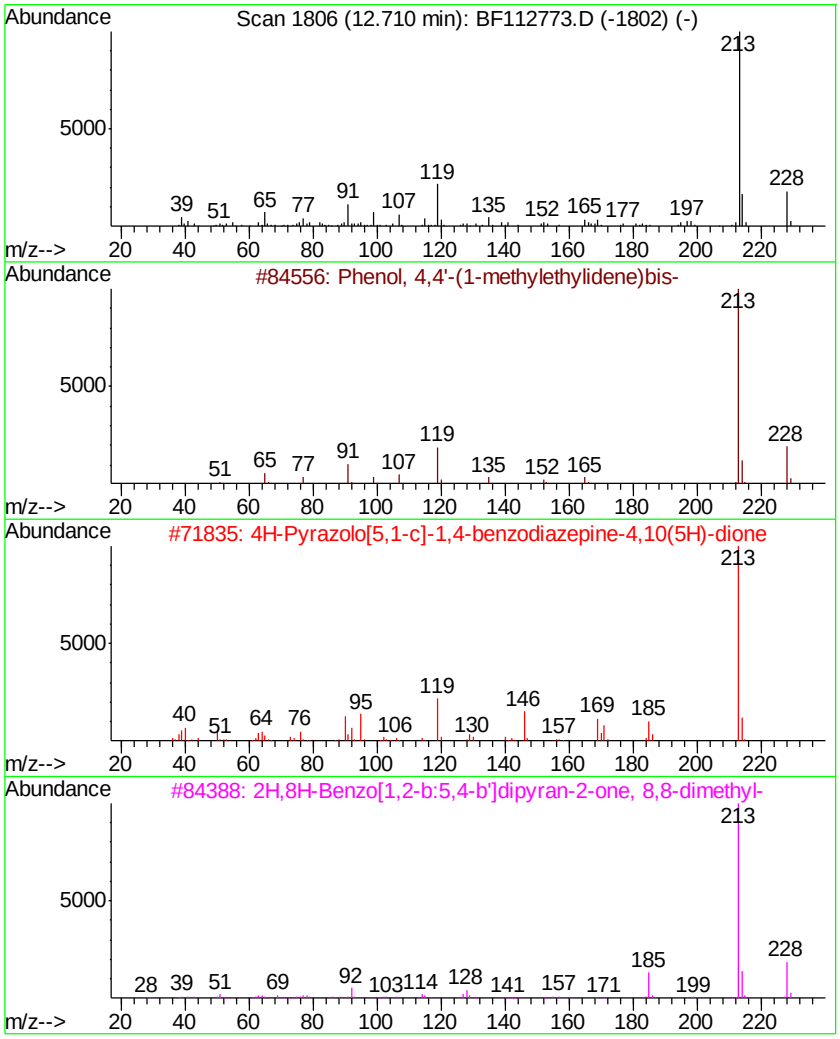
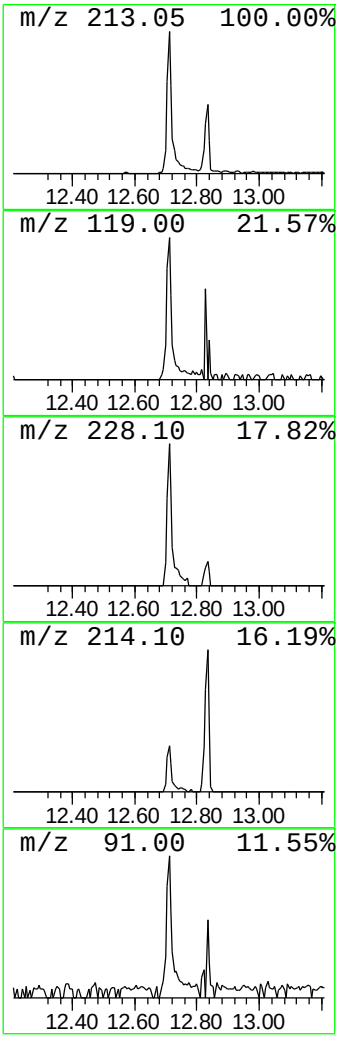
Peak Number 5 Phenol, 4,4'-(1-methylethyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	2.52 ng	146667	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	4H-Pyrazolo[5,1-c]-1,4-benzodiaz...	213	C11H7N3O2	1000277-20-1	64
3	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	53
4	6-Bromo-2-(methylamino)tropone	213	C8H8BrNO	1000241-43-1	50
5	2-Trifluoromethyl-5-hydroxyquino...	213	C10H6F3NO	041958-06-9	42





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
Data File : BF112773.D
Acq On : 28 Feb 2019 20:51
Operator : JU/SJ
Sample : K1650-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6(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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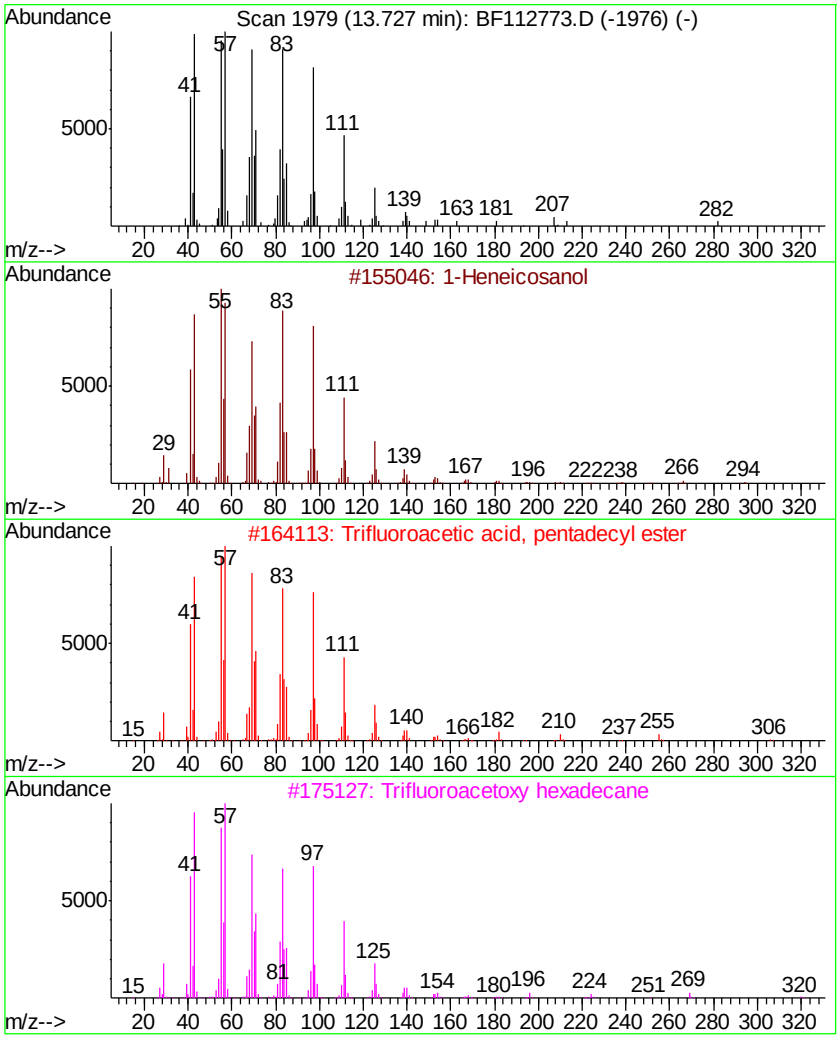
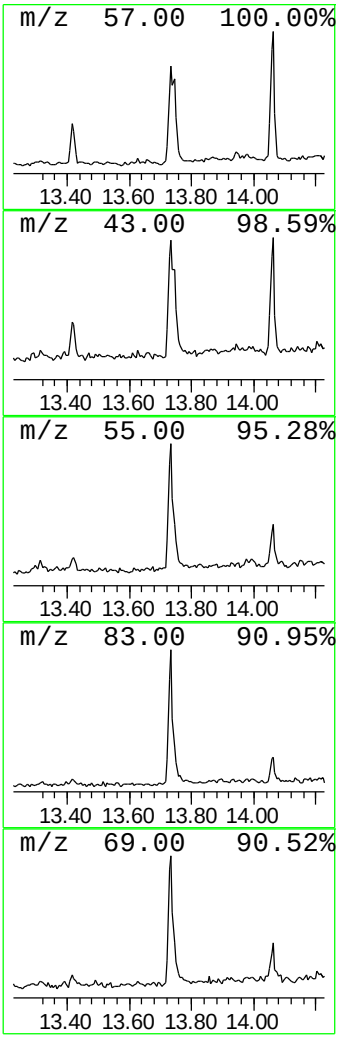
Peak Number 6 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.11 ng	239238	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
4	Behenic alcohol	326	C22H46O	000661-19-8	95
5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
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Operator : JU/SJ
Sample : K1650-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6(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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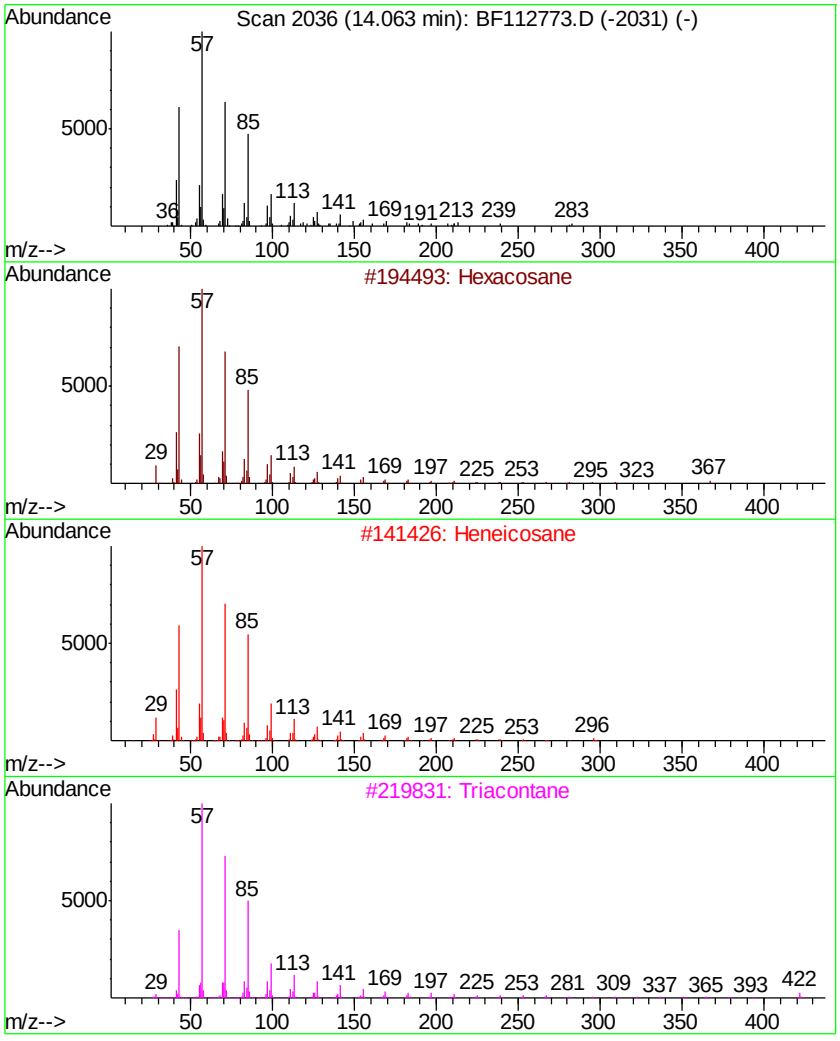
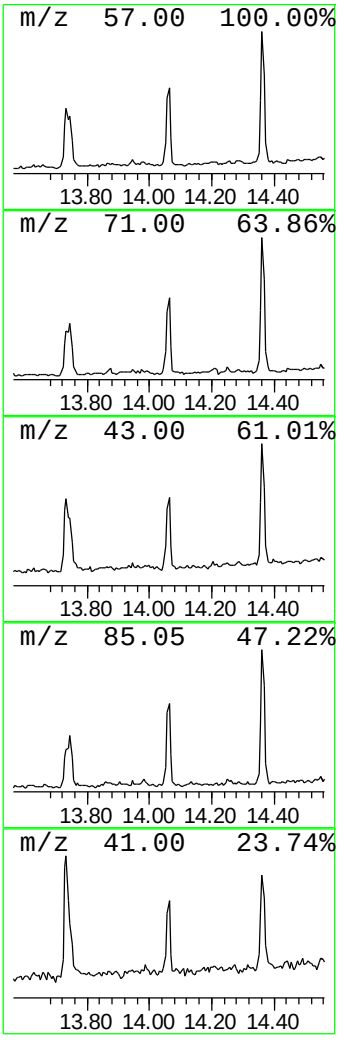
Peak Number 7 Hexacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.06	2.10 ng	122100	Chrysene-d12	13.87

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	Triacontane	422	C30H62	000638-68-6	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	90





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Instrument : BNA_F
ClientSampleId : B-6(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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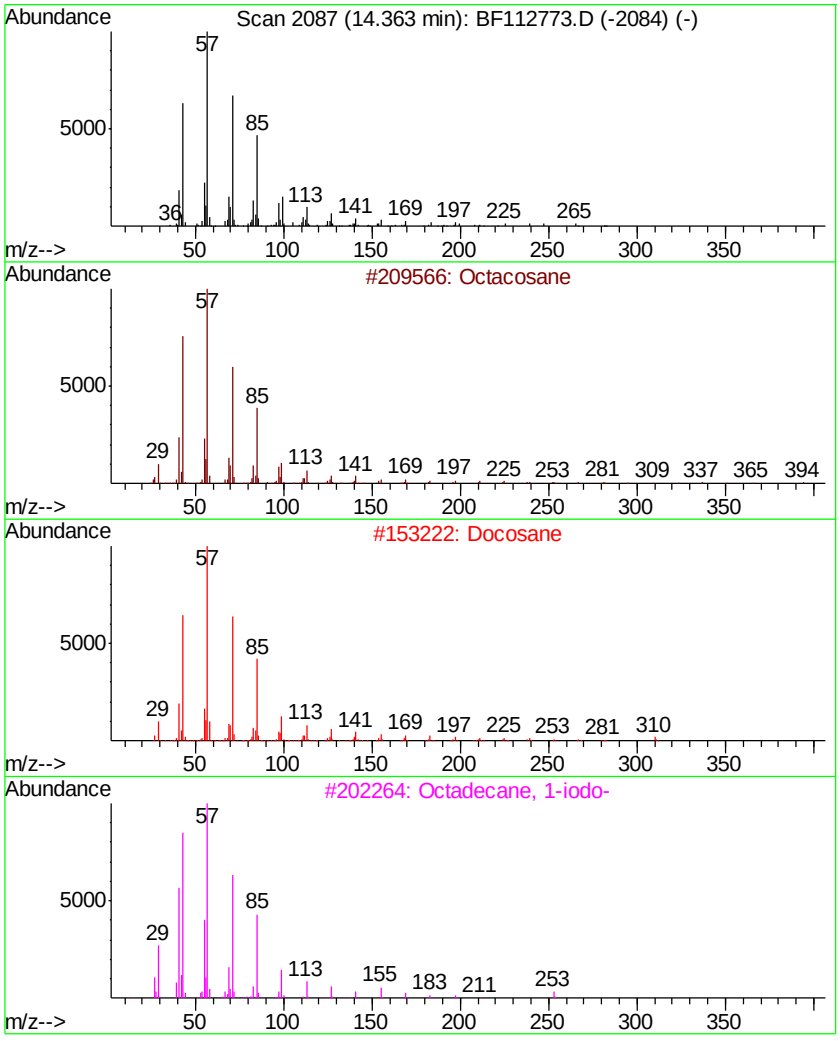
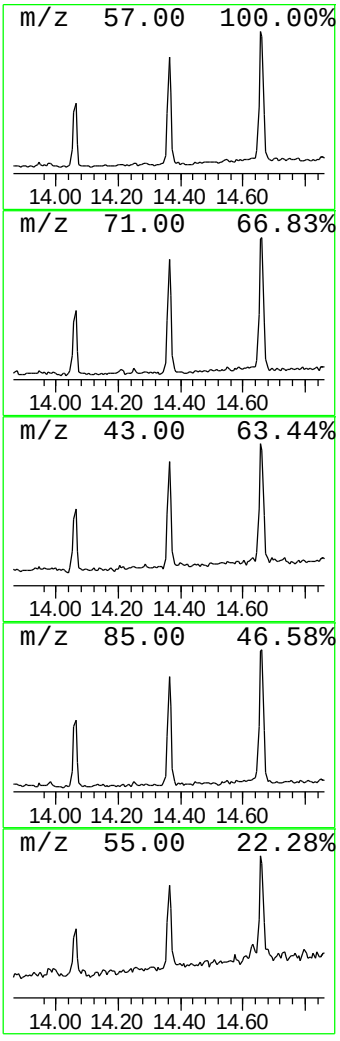
Peak Number 8 Octacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	2.79 ng	162182	Chrysene-d12	13.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Docosane	310	C22H46	000629-97-0	87
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Hexadecane	226	C16H34	000544-76-3	86





Library Search Compound Report

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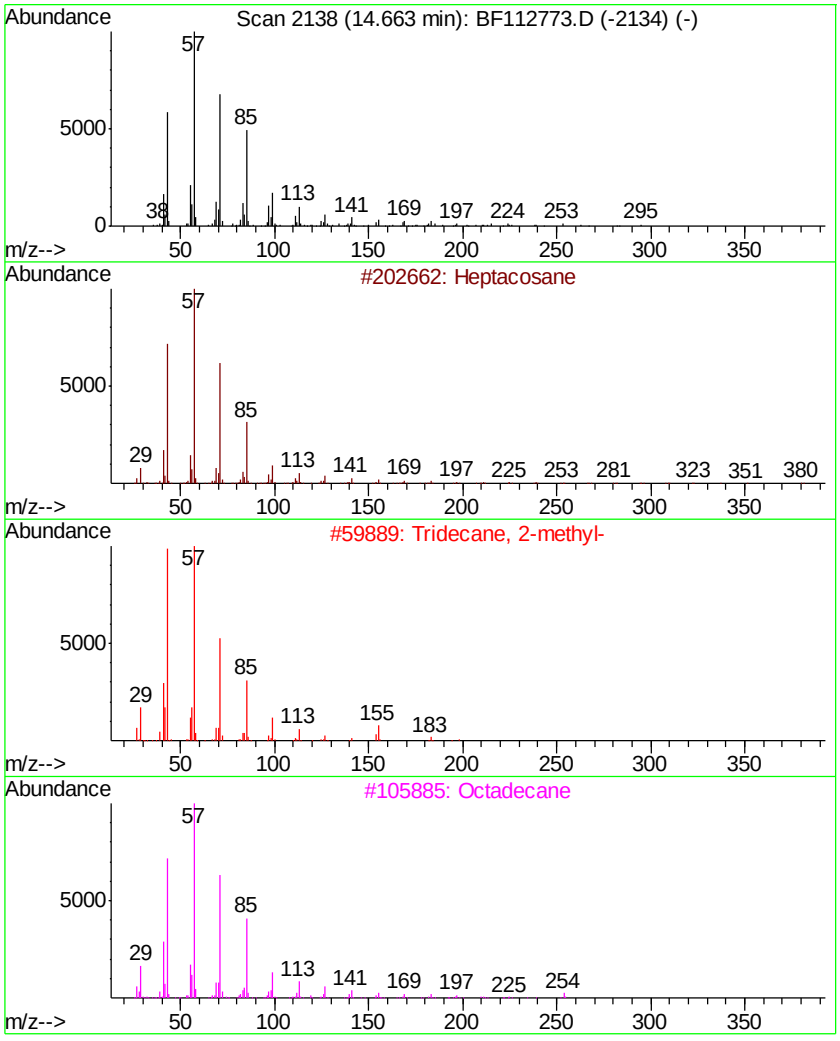
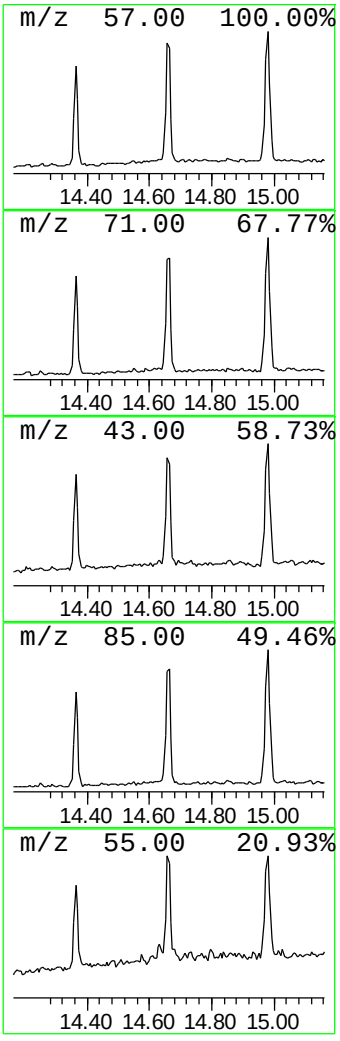
Peak Number 9 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.68 ng	217901	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Tridecane, 2-methyl-	198	C14H30	001560-96-9	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Eicosane	282	C20H42	000112-95-8	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 : B-6(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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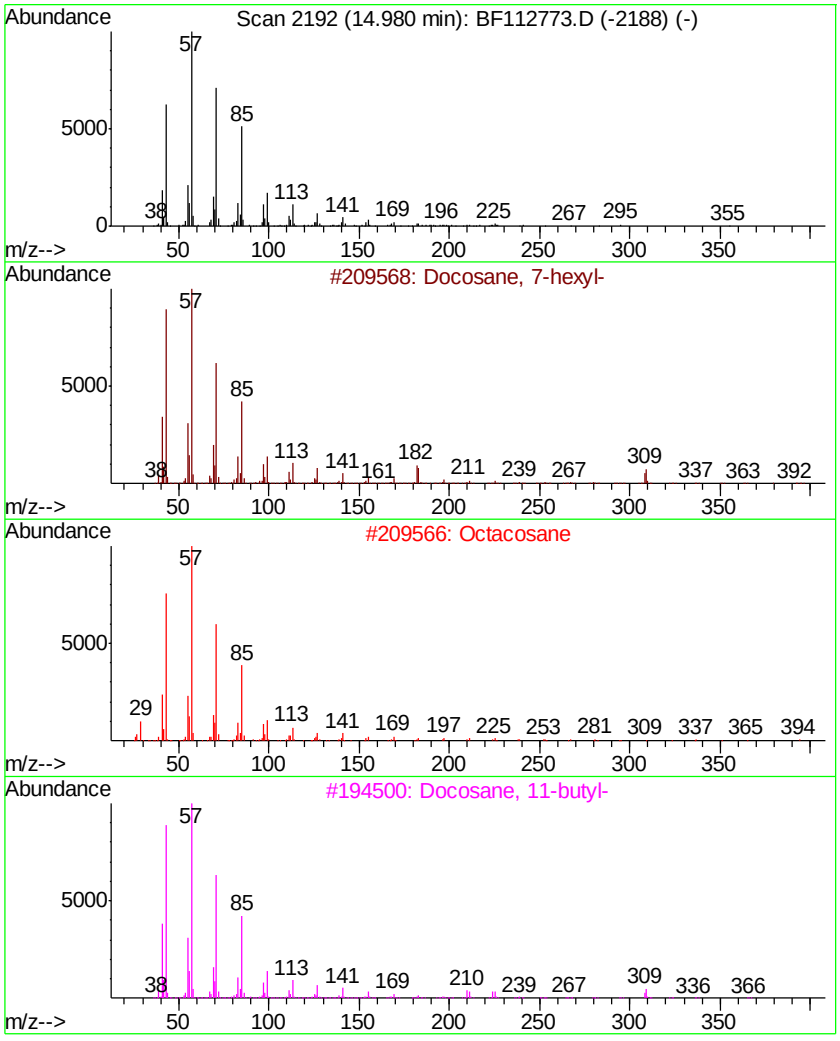
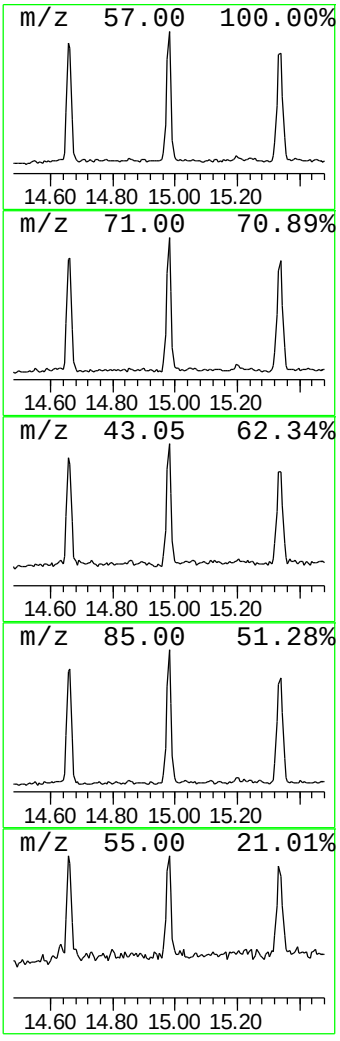
Peak Number 10 Docosane, 7-hexyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	4.40 ng	260796	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 7-hexyl-	394	C28H58	055373-86-9	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4	Octadecane	254	C18H38	000593-45-3	87
5	Heneicosane	296	C21H44	000629-94-7	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF022819\
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Operator : JU/SJ
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Misc :
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Instrument : BNA_F
ClientSampleId : B-6(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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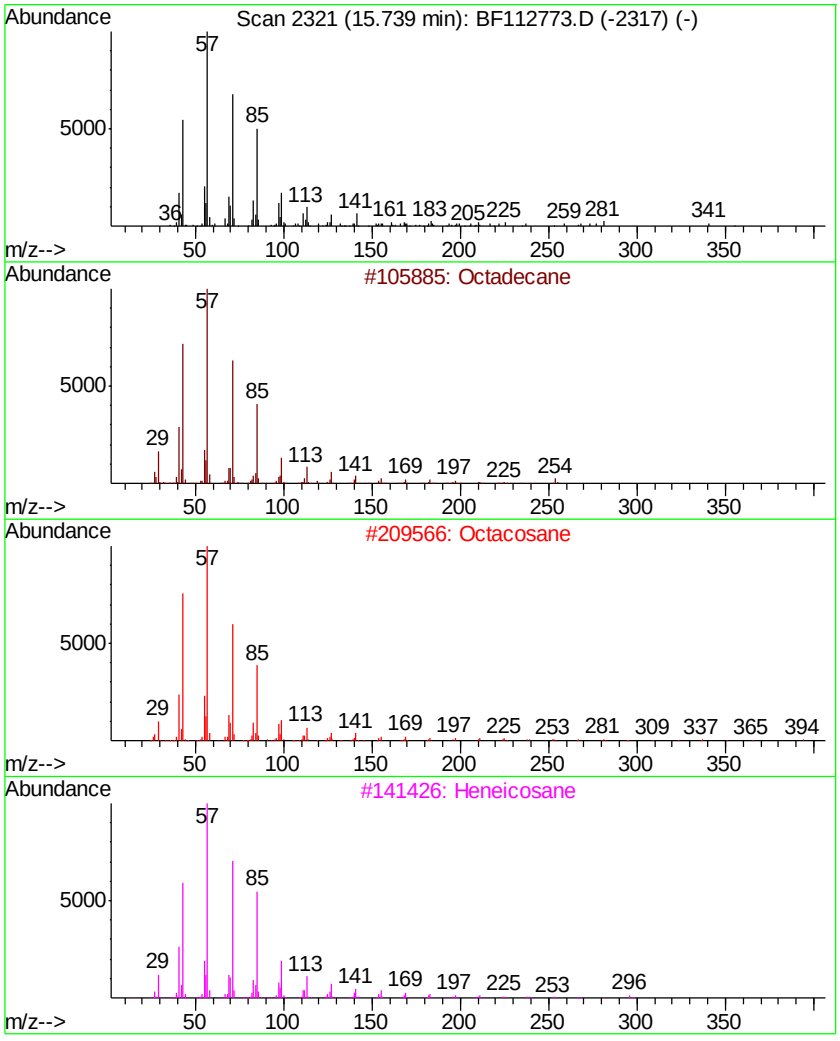
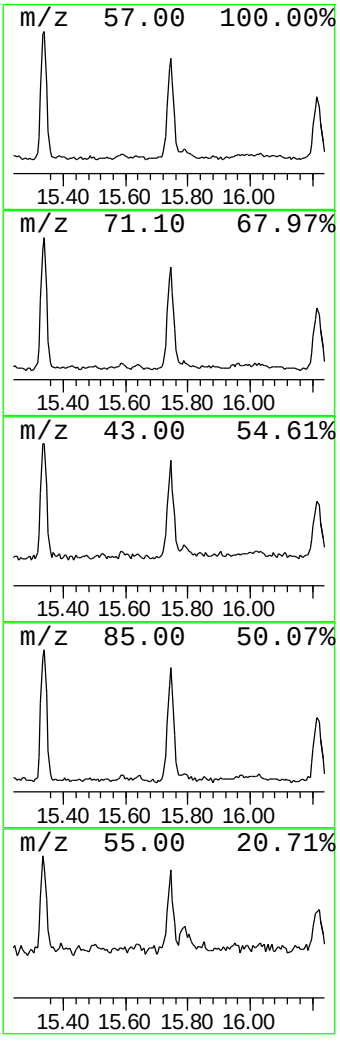
Peak Number 12 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.74	4.04 ng	239767	Perylene-d12	15.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	94
2	Octacosane	394	C28H58	000630-02-4	90
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF022819\
Data File : BF112773.D
Acq On : 28 Feb 2019 20:51
Operator : JU/SJ
Sample : K1650-13
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B-6(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
unknown6.51	6.51	82.7	ng	4551970	1	6.75	1100530	20.0
n-Hexadecanoic acid	11.79	6.1	ng	461556	4	11.25	1519690	20.0
Octadecanoic acid	12.57	3.3	ng	194240	5	13.87	1162970	20.0
Phenol, 4,4'-(1-m...	12.71	2.5	ng	146667	5	13.87	1162970	20.0
1-Heneicosanol	13.73	4.1	ng	239238	5	13.87	1162970	20.0
Hexacosane	14.06	2.1	ng	122100	5	13.87	1162970	20.0
Octacosane	14.36	2.8	ng	162182	5	13.87	1162970	20.0
Heptacosane	14.66	3.7	ng	217901	6	15.28	1185800	20.0
Docosane, 7-hexyl-	14.98	4.4	ng	260796	6	15.28	1185800	20.0
Octadecane	15.74	4.0	ng	239767	6	15.28	1185800	20.0