LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF041619\
Data File : BF113792.D
Acq On : 16 Apr 2019 14:29
Operator : JU/SJ
Sample : K2414-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-044

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-BF040319.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	5.293	542	545	579	rBV	2162577	2994277	96.03%	11.121%
2	6.334	718	722	738	rBV	2429286	3076750	98.68%	11.427%
3	6.451	738	742	765	rVB	3097818	3117990	100.00%	11.581%
4	6.669	776	779	790	rVB	712101	688084	22.07%	2.556%
5	6.828	802	806	827	rBV	2586296	2352632	75.45%	8.738%
6	7.240	872	876	907	rBV	1730587	1975953	63.37%	7.339%
7	7.957	994	998	1019	rBV	689137	851883	27.32%	3.164%
8	9.028	1176	1180	1194	rBV	3324519	3076591	98.67%	11.427%
9	9.428	1245	1248	1261	rBV	298960	332487	10.66%	1.235%
10	9.704	1291	1295	1307	rBV	936696	878736	28.18%	3.264%
11	10.498	1426	1430	1446	rBV	1463270	1675934	53.75%	6.225%
12	11.186	1544	1547	1566	rBV	657686	824396	26.44%	3.062%
13	11.727	1636	1639	1650	rBV3	62695	117421	3.77%	0.436%
14	12.510	1769	1772	1782	rBV3	39224	83933	2.69%	0.312%
15	12.769	1812	1816	1828	rVB	2412255	2184657	70.07%	8.114%
16	13.669	1965	1969	1975	rVB	31940	32927	1.06%	0.122%
17	13.827	1992	1996	2006	rBV	725362	821910	26.36%	3.053%
18	13.980	2019	2022	2027	rVB	49400	46709	1.50%	0.173%
19	14.286	2069	2074	2077	rBV	79932	77298	2.48%	0.287%
20	14.580	2120	2124	2132	rVB	99724	104488	3.35%	0.388%
21	14.886	2172	2176	2184	rVB	167554	181430	5.82%	0.674%
22	15.239	2230	2236	2248	rBV	680772	1014193	32.53%	3.767%
23	15.621	2297	2301	2309	rVB	91604	124727	4.00%	0.463%
24	16.074	2373	2378	2389	rVB3	49774	88350	2.83%	0.328%
25	16.333	2419	2422	2430	rVB6	27039	44587	1.43%	0.166%
26	18.921	2855	2862	2870	rVB8	55762	155940	5.00%	0.579%

Sum of corrected areas: 26924283

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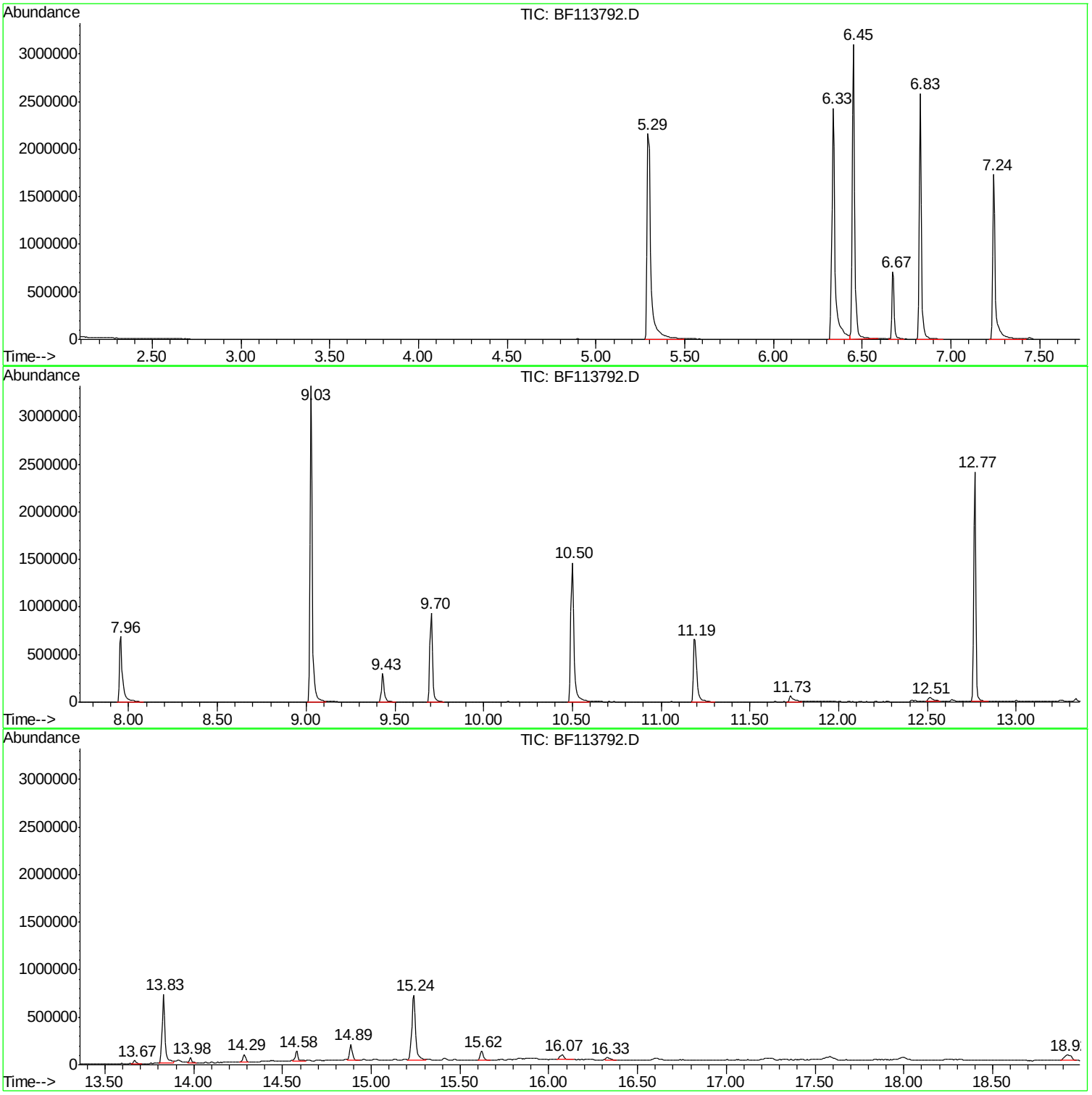
Instrument : BNA_F
ClientSampleId : FK-PS-01-044

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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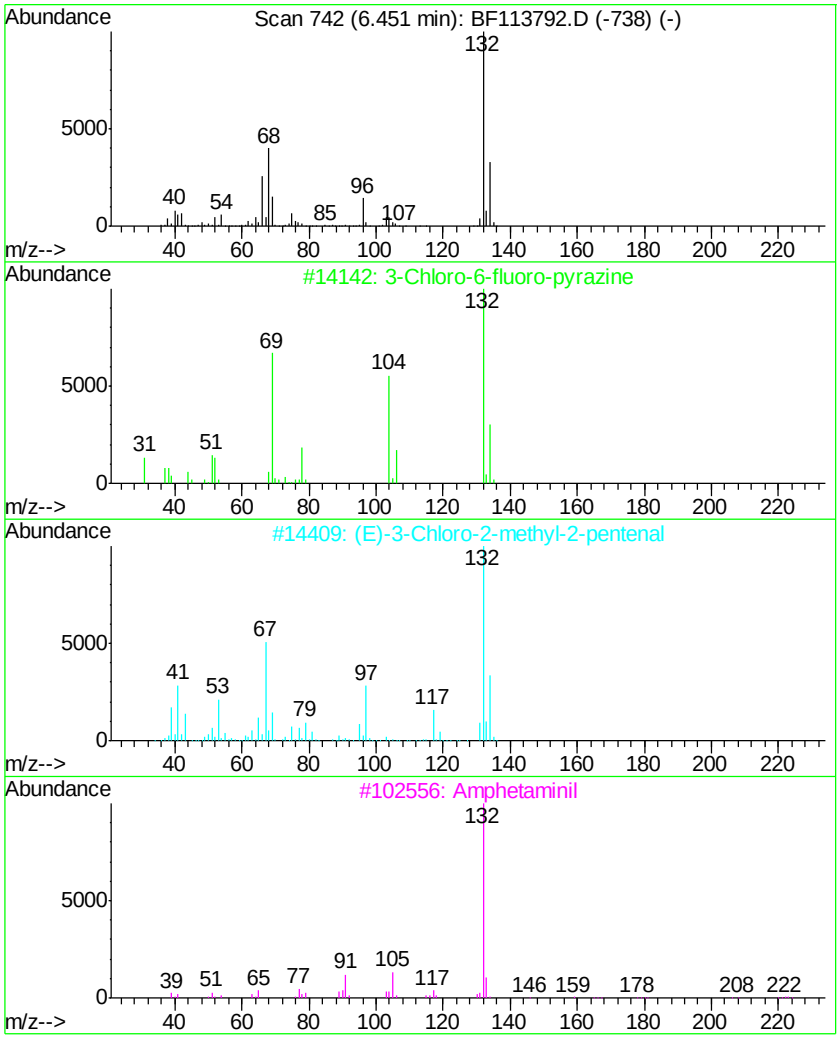
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

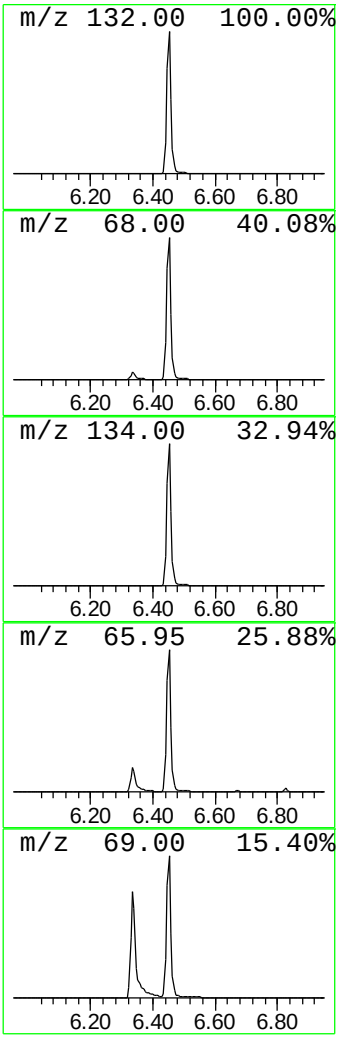
****

Peak Number 1 unknown6.45 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	90.63 ng	3117990	1,4-Dichlorobenzene-d4	6.67

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	Amphetaminil	250	C17H18N2	017590-01-1	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





Library Search Compound Report

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Data File : BF113792.D
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Operator : JU/SJ
Sample : K2414-01
Misc :
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Instrument : BNA_F
ClientSampleId : FK-PS-01-044

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

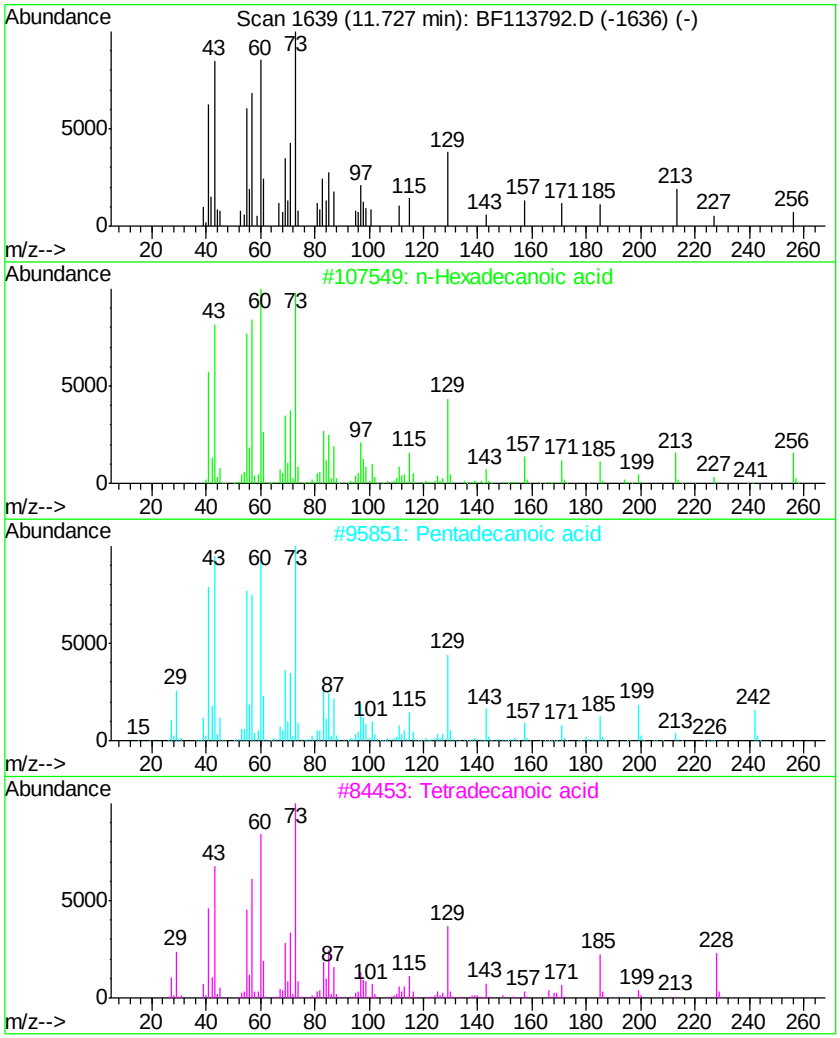
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

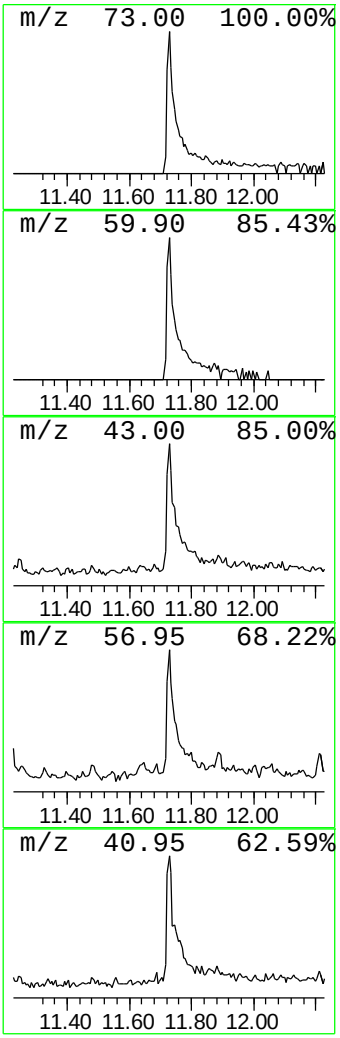
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.73	2.85 ng	117421	Phenanthrene-d10	11.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF041619\
Data File : BF113792.D
Acq On : 16 Apr 2019 14:29
Operator : JU/SJ
Sample : K2414-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-044

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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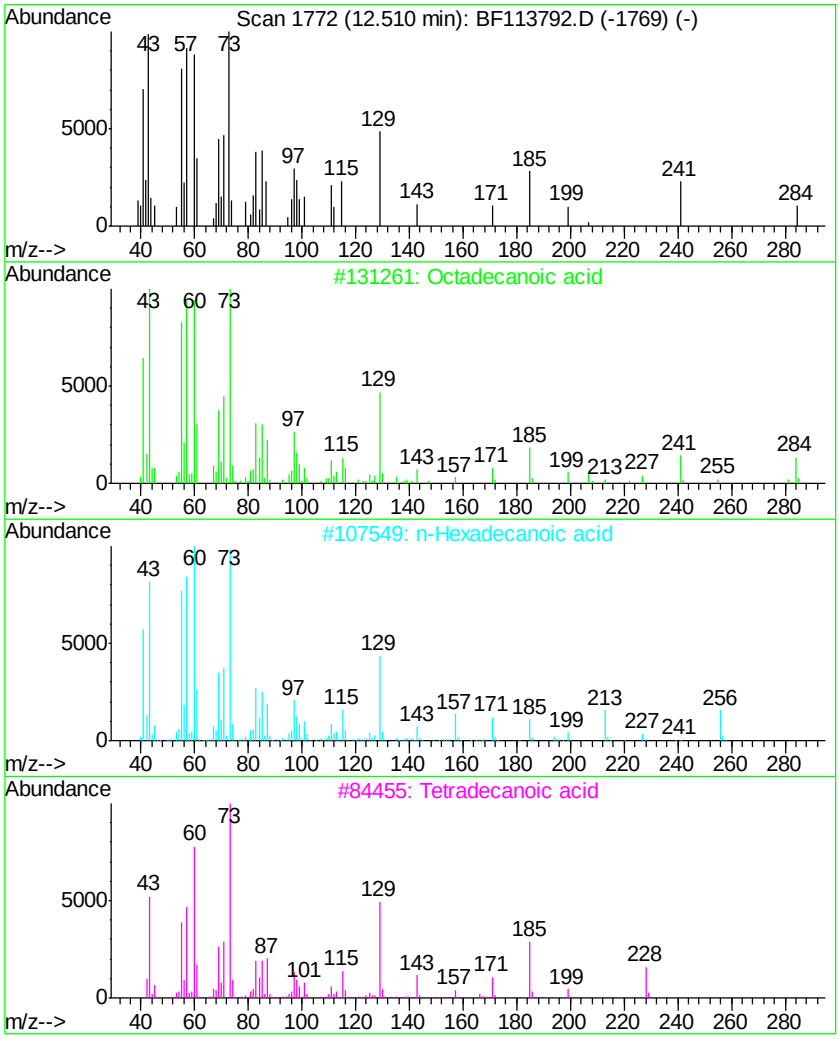
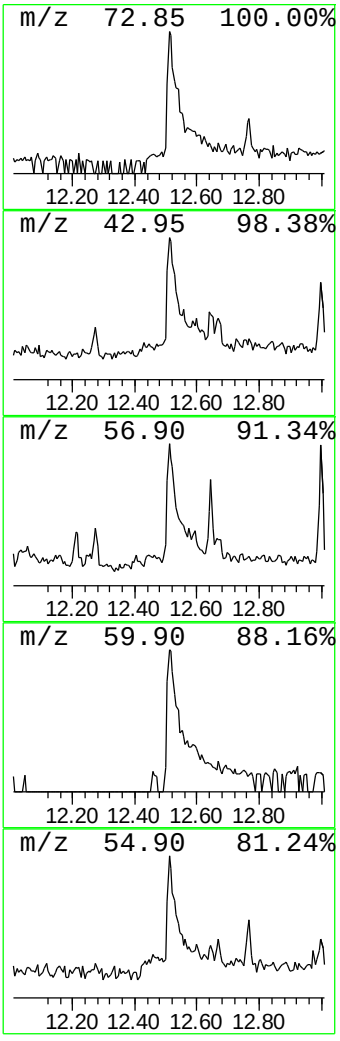
Peak Number 4 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.51	2.04 ng	83933	Chrysene-d12	13.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	64
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4	n-Decanoic acid	172	C10H20O2	000334-48-5	38
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF041619\
Data File : BF113792.D
Acq On : 16 Apr 2019 14:29
Operator : JU/SJ
Sample : K2414-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-044

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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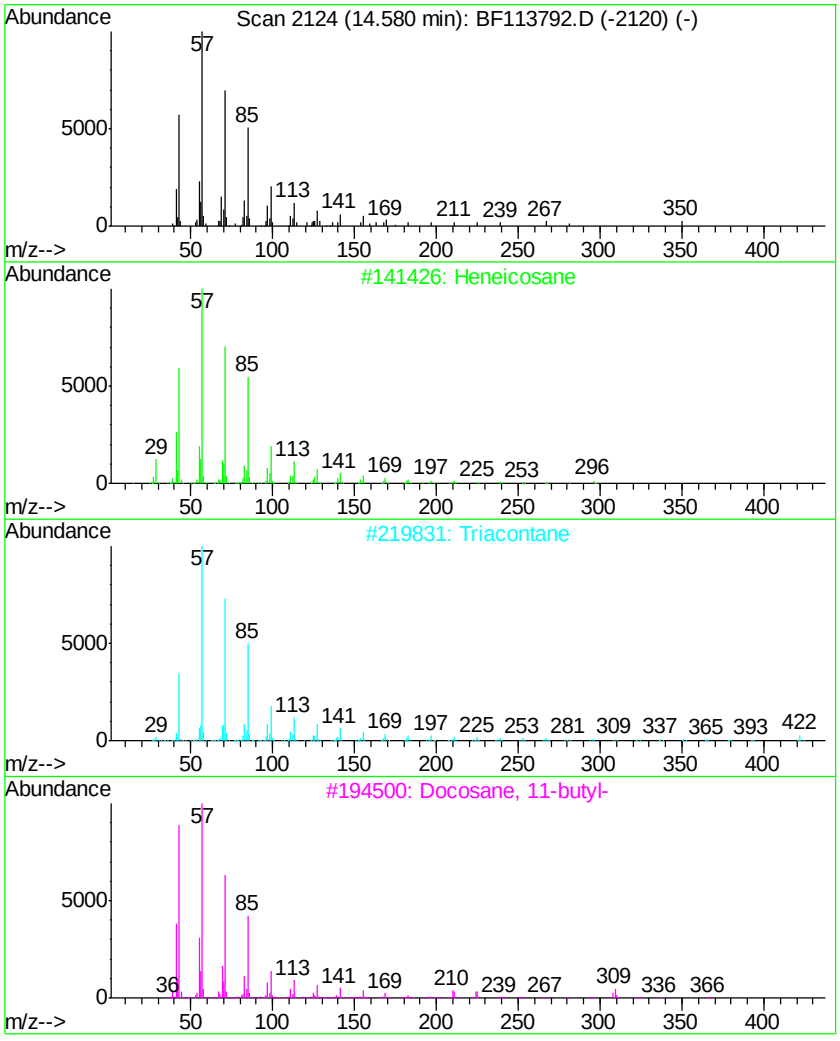
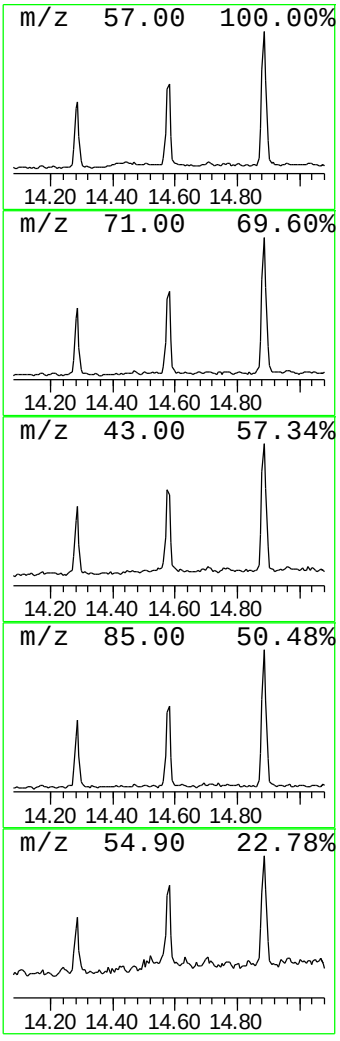
Peak Number 5 Heneicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.58	2.06 ng	104488	Perylene-d12	15.24

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	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

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Data File : BF113792.D
Acq On : 16 Apr 2019 14:29
Operator : JU/SJ
Sample : K2414-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FK-PS-01-044

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.M
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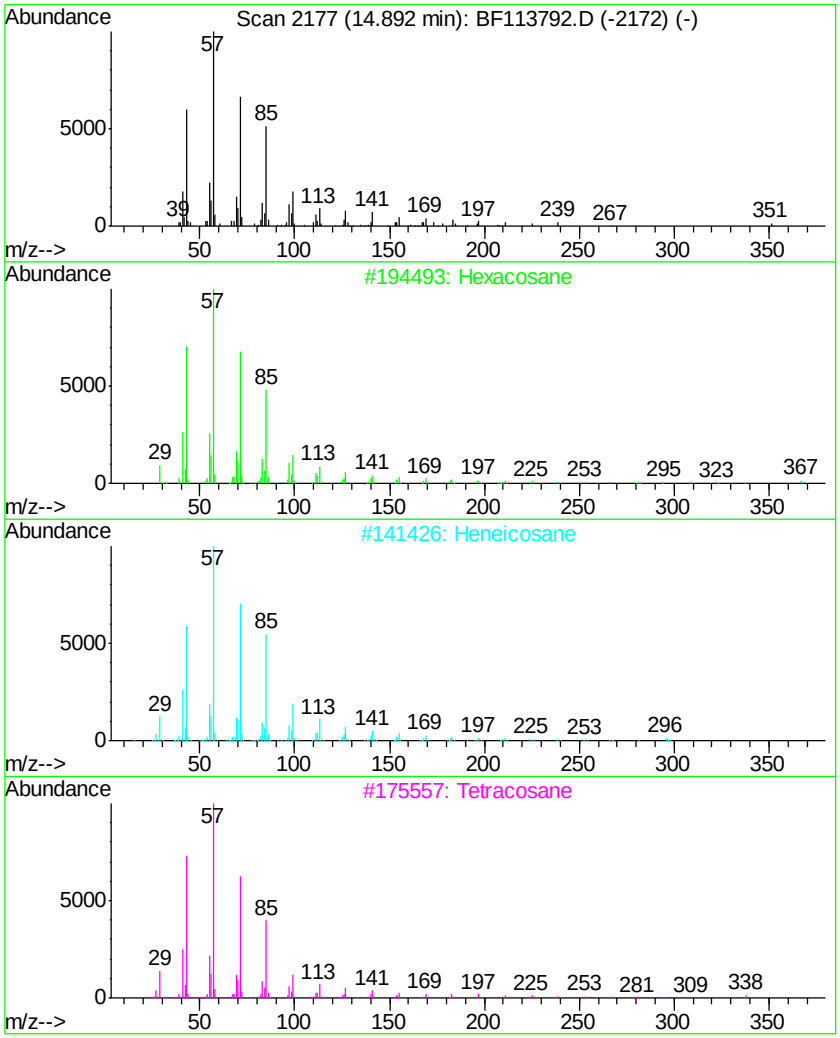
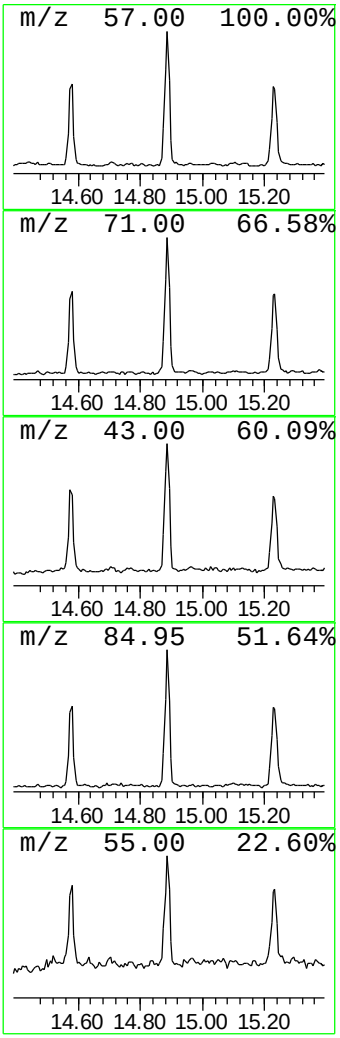
****

Peak Number 6 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	3.58 ng	181430	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Docosane	310	C22H46	000629-97-0	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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Misc :
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Instrument : BNA_F
ClientSampleId : FK-PS-01-044

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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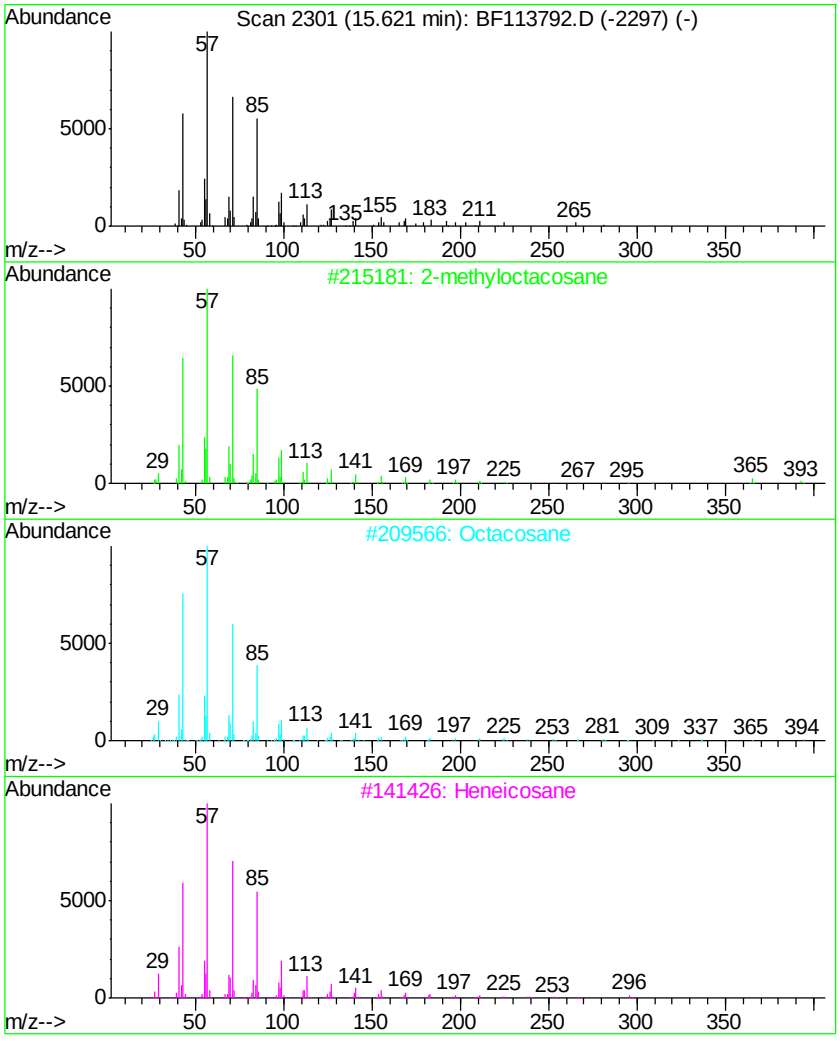
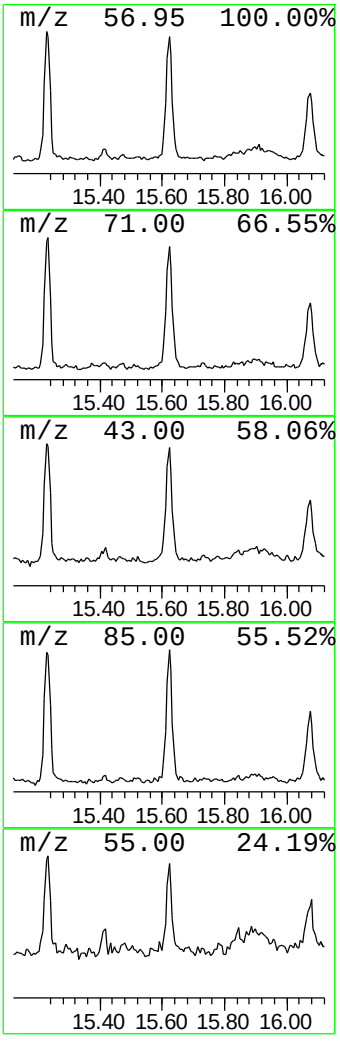
Peak Number 7 2-methyloctacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.62	2.46 ng	124727	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Hexacosane	366	C26H54	000630-01-3	90
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90





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Instrument : BNA_F
ClientSampleId : FK-PS-01-044

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF040319.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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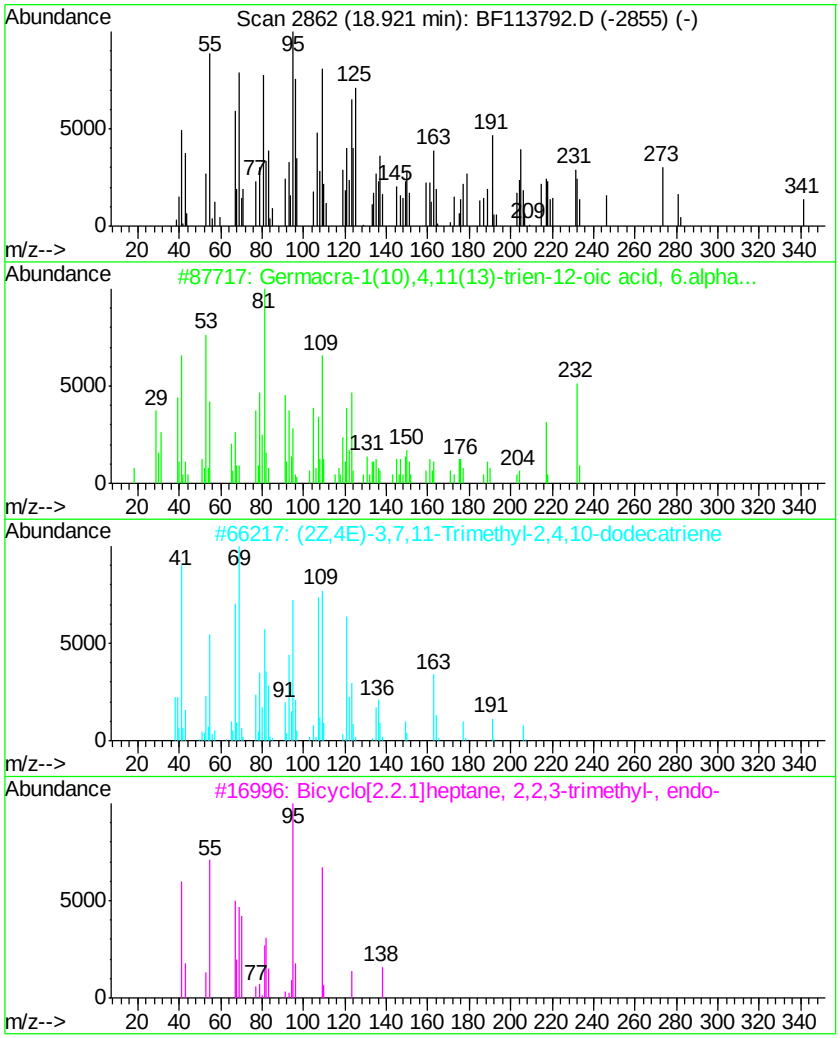
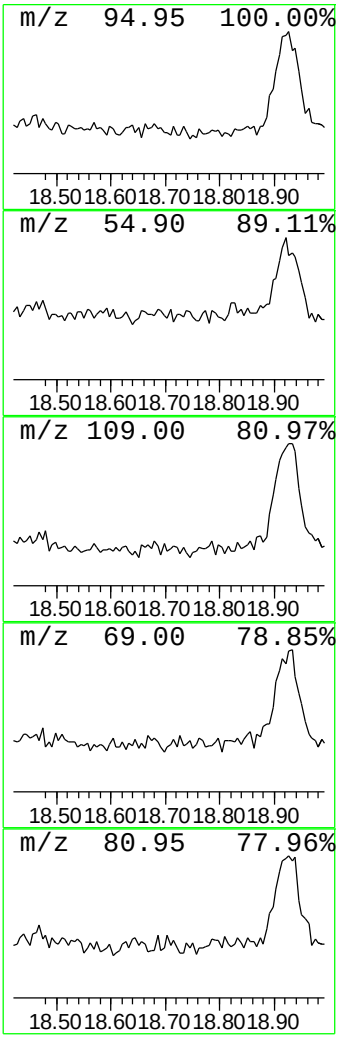
Peak Number 8 unknown18.92 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.92	3.08 ng	155940	Perylene-d12	15.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Germacra-1(10),4,11(13)-trien-12...	232	C15H20O2	000553-21-9	45
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	41
3	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	38
4	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	38
5	[1,3,4]Oxadiazole, 2-amino-5-(4-...	179	C8H6FN3O	1000316-48-2	25





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\DATABASE\NIST11.L
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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.45	6.45	90.6	ng	3117990	1	6.67	688084	20.0
n-Hexadecanoic acid	11.73	2.9	ng	117421	4	11.19	824396	20.0
Octadecanoic acid	12.51	2.0	ng	83933	5	13.83	821910	20.0
Heneicosane	14.58	2.1	ng	104488	6	15.24	1014190	20.0
Hexacosane	14.89	3.6	ng	181430	6	15.24	1014190	20.0
2-methyloctacosane	15.62	2.5	ng	124727	6	15.24	1014190	20.0
unknown18.92	18.92	3.1	ng	155940	6	15.24	1014190	20.0