LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061319\
Data File : BF115009.D
Acq On : 13 Jun 2019 18:44
Operator : HP/JU
Sample : K3345-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-MW-11_061119

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-BF061219.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	5.251	534	538	542	rBV	3234133	3029054	36.12%	5.275%
2	6.281	709	713	722	rBV	2144564	2106019	25.11%	3.668%
3	6.416	731	736	739	rBV	5703833	5542272	66.08%	9.652%
4	6.645	771	775	779	rBV	1977427	1636332	19.51%	2.850%
5	6.804	797	802	805	rBV	5855079	5550047	66.17%	9.665%
6	7.210	865	871	874	rBV	4077821	4478214	53.39%	7.799%
7	7.928	988	993	996	rBV	2339260	2109668	25.15%	3.674%
8	9.004	1170	1176	1179	rBV	7453858	8387009	100.00%	14.606%
9	9.675	1284	1290	1299	rBV	2724213	2446286	29.17%	4.260%
10	10.457	1418	1423	1427	rBV	4370471	4666969	55.65%	8.128%
11	11.145	1536	1540	1544	rBV	2700400	2502038	29.83%	4.357%
12	11.692	1630	1633	1645	rBV2	275141	365621	4.36%	0.637%
13	12.474	1763	1766	1778	rBV	140309	202298	2.41%	0.352%
14	12.733	1805	1810	1813	rBV	7179180	8118232	96.80%	14.138%
15	13.698	1967	1974	1982	rBV10	44572	159056	1.90%	0.277%
16	13.768	1982	1986	1996	rVB	2225346	2001739	23.87%	3.486%
17	14.262	2067	2070	2073	rBV	140060	118863	1.42%	0.207%
18	14.557	2116	2120	2124	rVB	265339	248524	2.96%	0.433%
19	14.862	2166	2172	2179	rBV	395520	489458	5.84%	0.852%
20	15.145	2215	2220	2225	rBV	1443395	1647828	19.65%	2.870%
21	15.198	2225	2229	2235	rVB	473879	608938	7.26%	1.060%
22	15.586	2289	2295	2304	rBV	396900	585340	6.98%	1.019%
23	16.033	2365	2371	2380	rBV	183861	327399	3.90%	0.570%
24	16.551	2454	2459	2466	rBV3	50769	94681	1.13%	0.165%

Sum of corrected areas: 57421885

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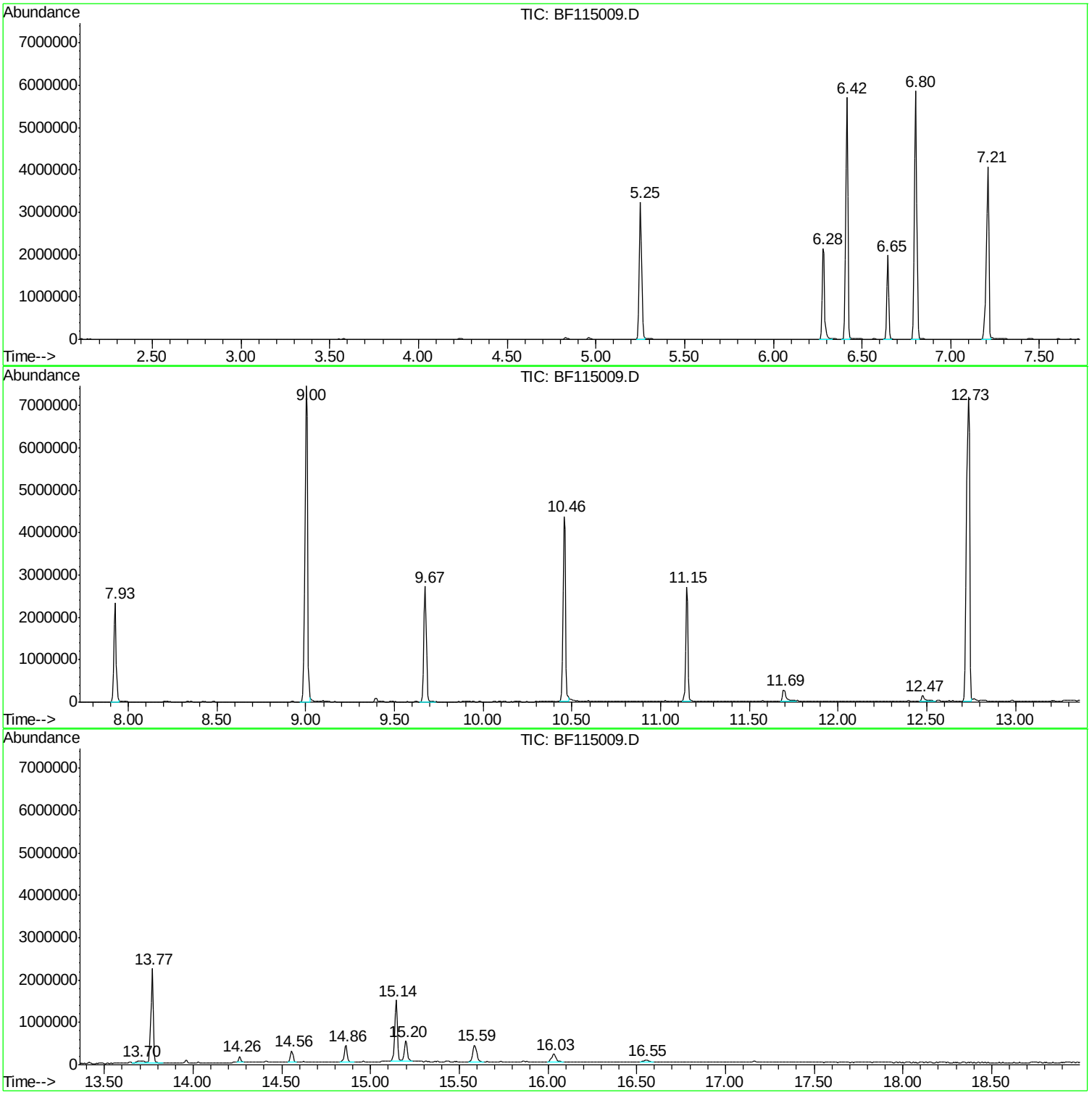
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
C-MW-11_061119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061319\
Data File : BF115009.D
Acq On : 13 Jun 2019 18:44
Operator : HP/JU
Sample : K3345-04
Misc :
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Instrument : BNA_F
ClientSampleId : C-MW-11_061119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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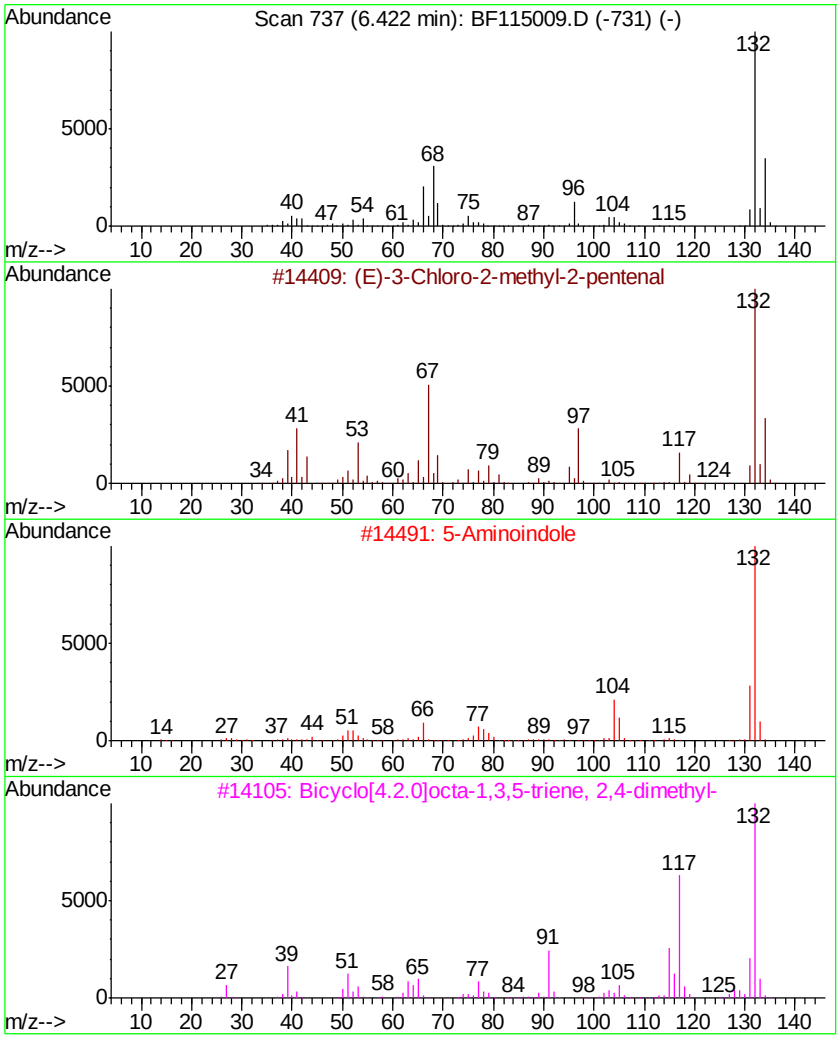
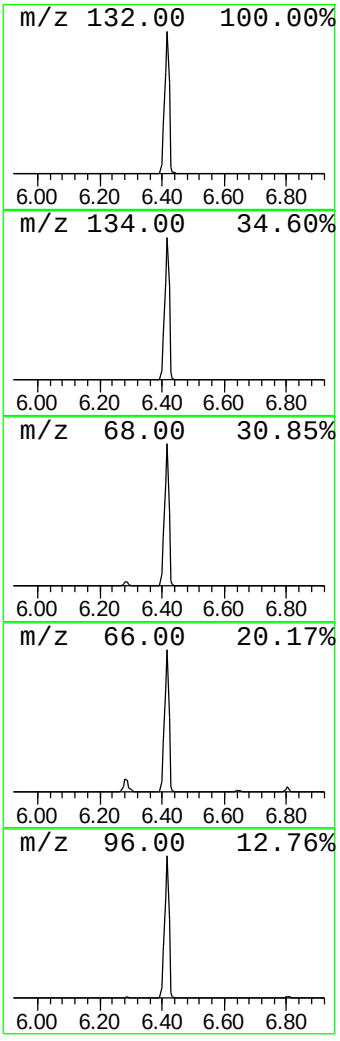
Peak Number 1 unknown6.42 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.42	67.74 ng	5542270	1,4-Dichlorobenzene-d4	6.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Data File : BF115009.D
Acq On : 13 Jun 2019 18:44
Operator : HP/JU
Sample : K3345-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-MW-11_061119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.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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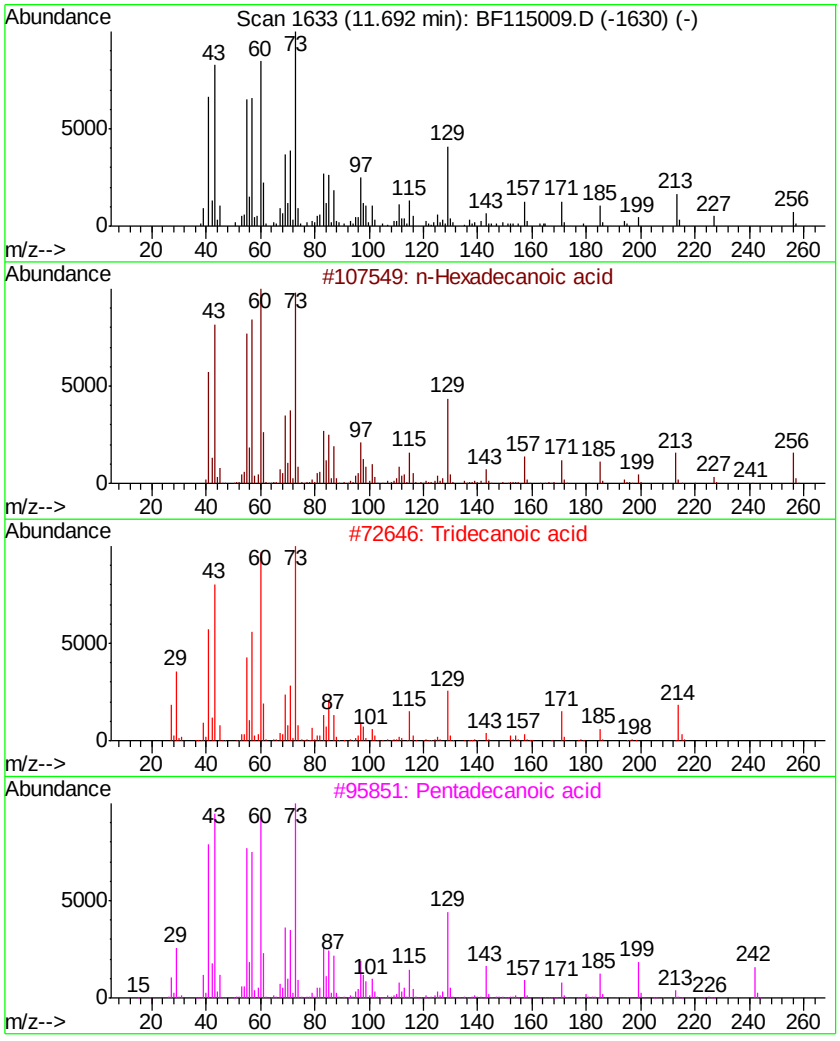
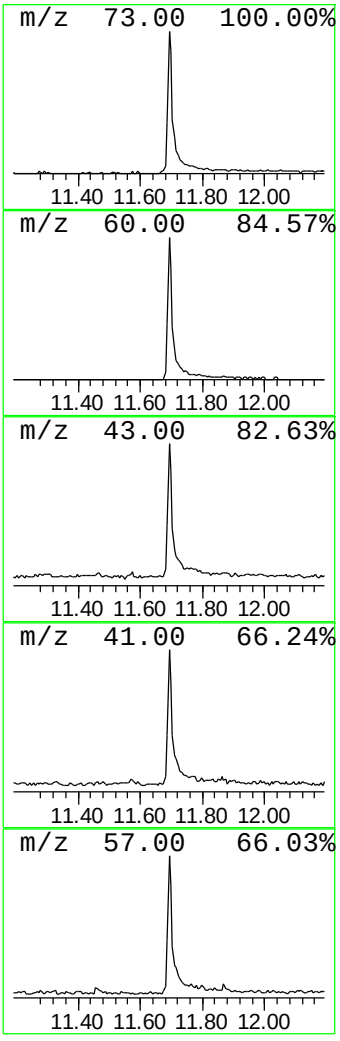
Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	2.92 ng	365621	Phenanthrene-d10	11.15

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061319\
Data File : BF115009.D
Acq On : 13 Jun 2019 18:44
Operator : HP/JU
Sample : K3345-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-MW-11_061119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.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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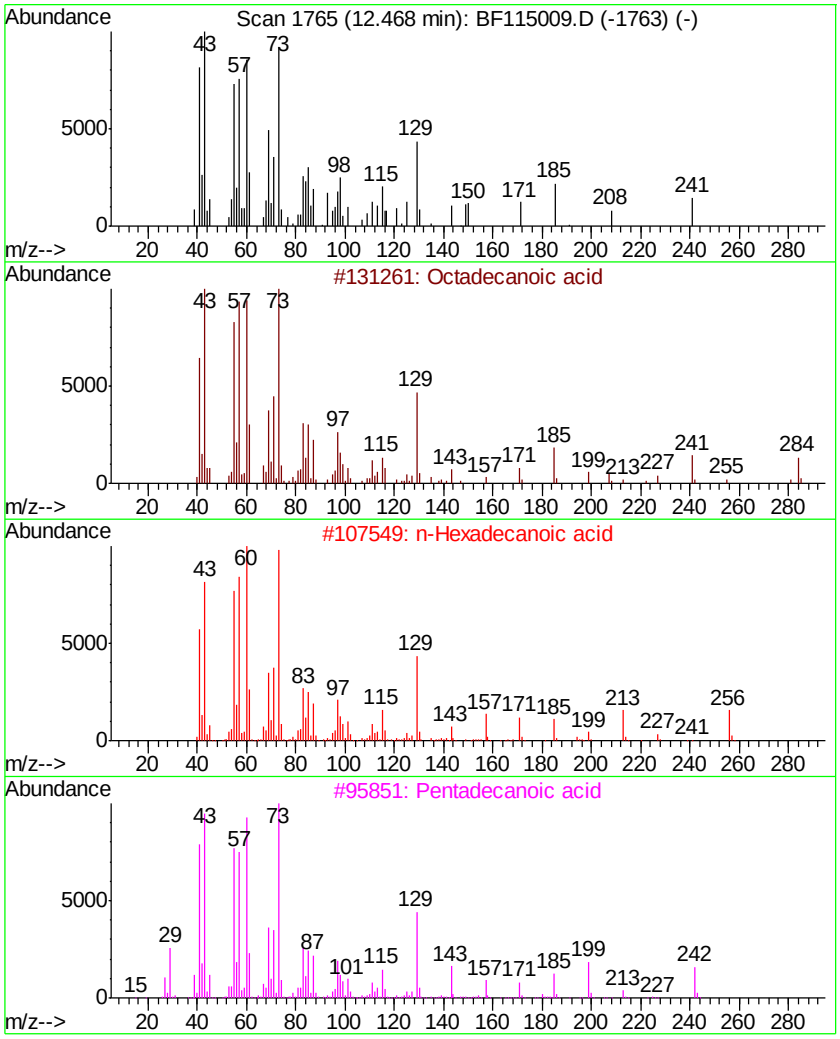
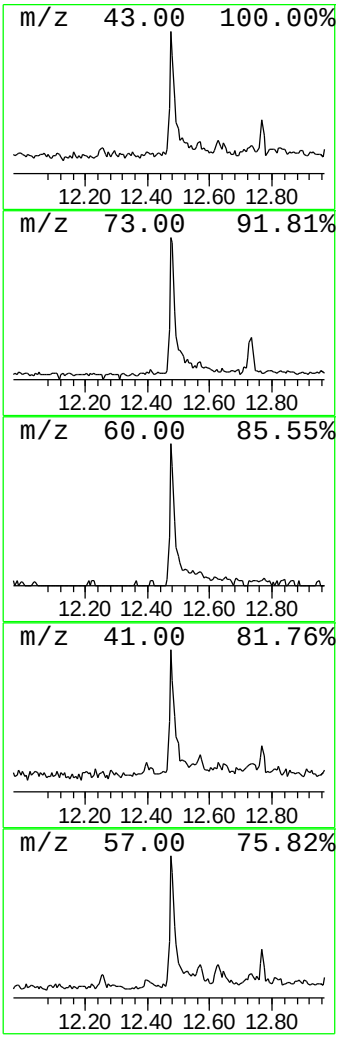
Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	2.02 ng	202298	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061319\
Data File : BF115009.D
Acq On : 13 Jun 2019 18:44
Operator : HP/JU
Sample : K3345-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-MW-11_061119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.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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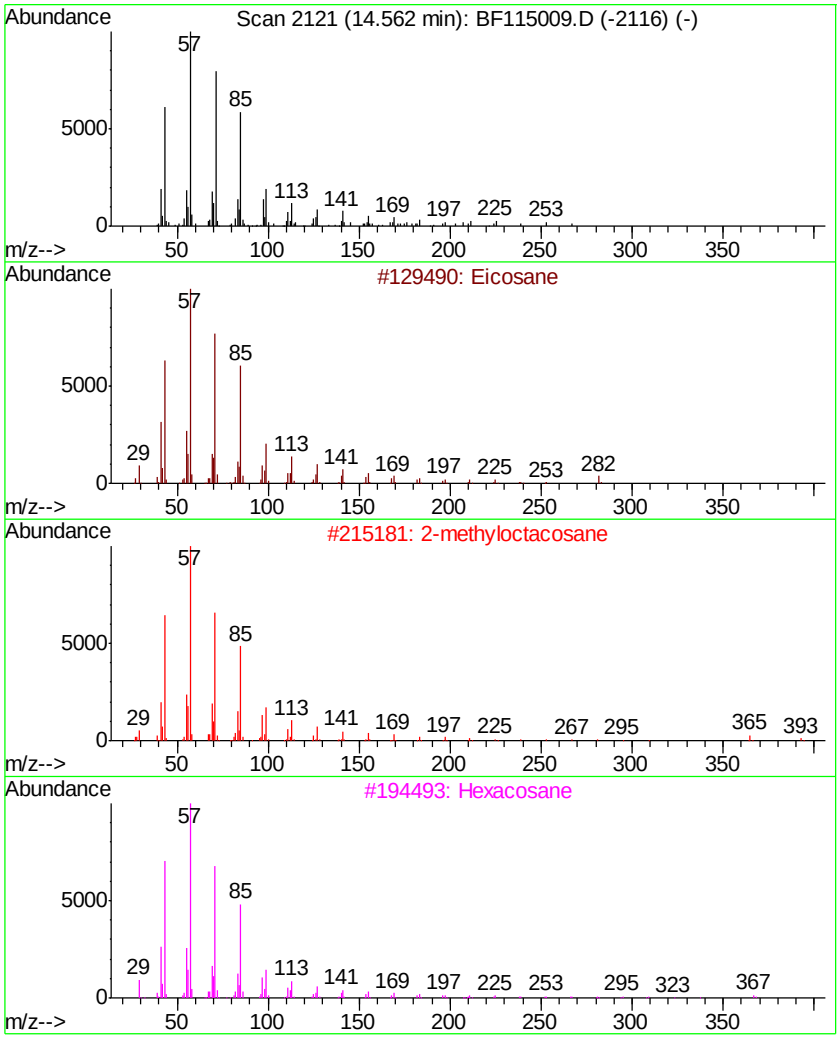
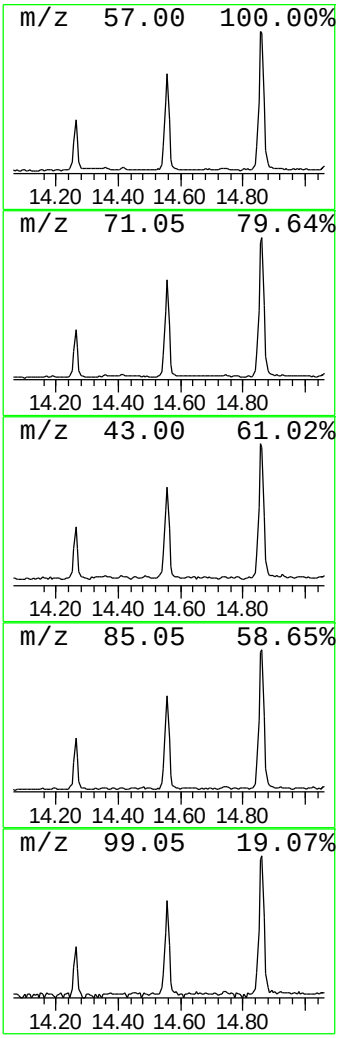
Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	3.02 ng	248524	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Triacontane	422	C30H62	000638-68-6	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061319\
Data File : BF115009.D
Acq On : 13 Jun 2019 18:44
Operator : HP/JU
Sample : K3345-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-MW-11_061119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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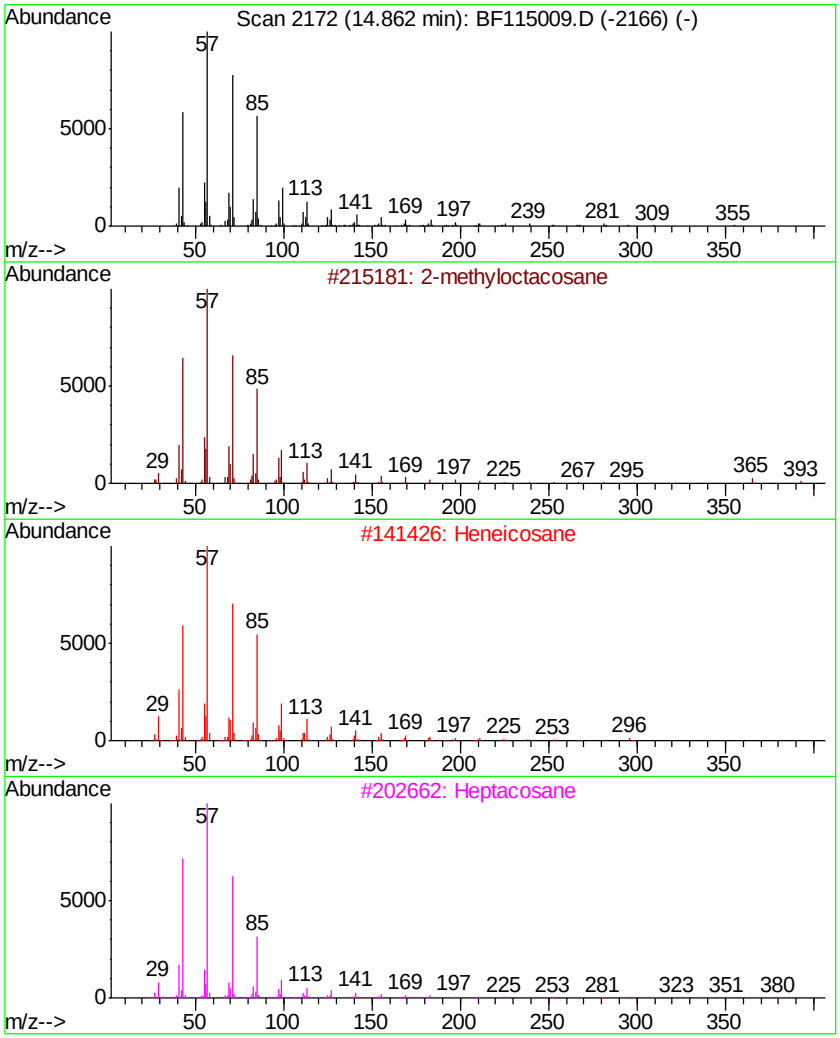
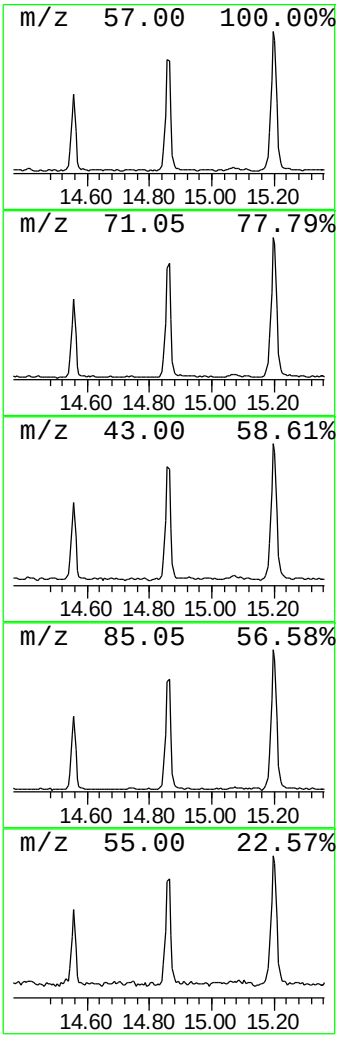
Peak Number 6 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	5.94 ng	489458	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptacosane	380	C27H56	000593-49-7	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF061319\
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Misc :
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Instrument : BNA_F
ClientSampleId : C-MW-11_061119

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061219.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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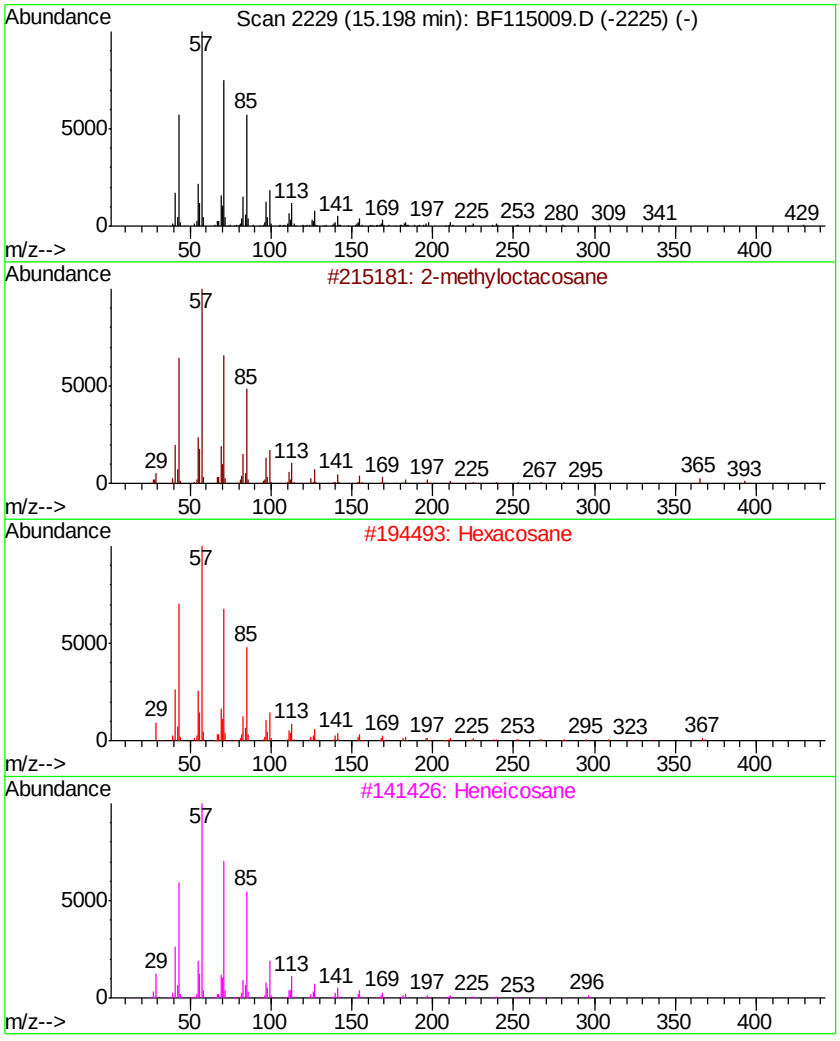
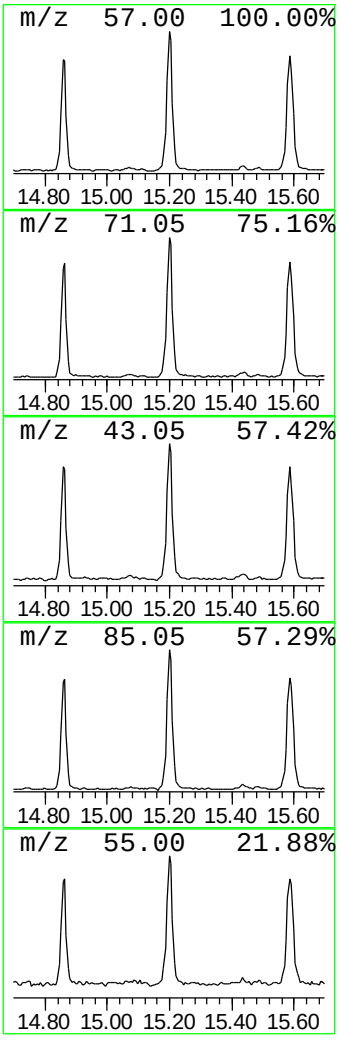
Peak Number 7 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	7.39 ng	608938	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
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	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





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Sample : K3345-04
Misc :
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Instrument : BNA_F
ClientSampleId : C-MW-11_061119

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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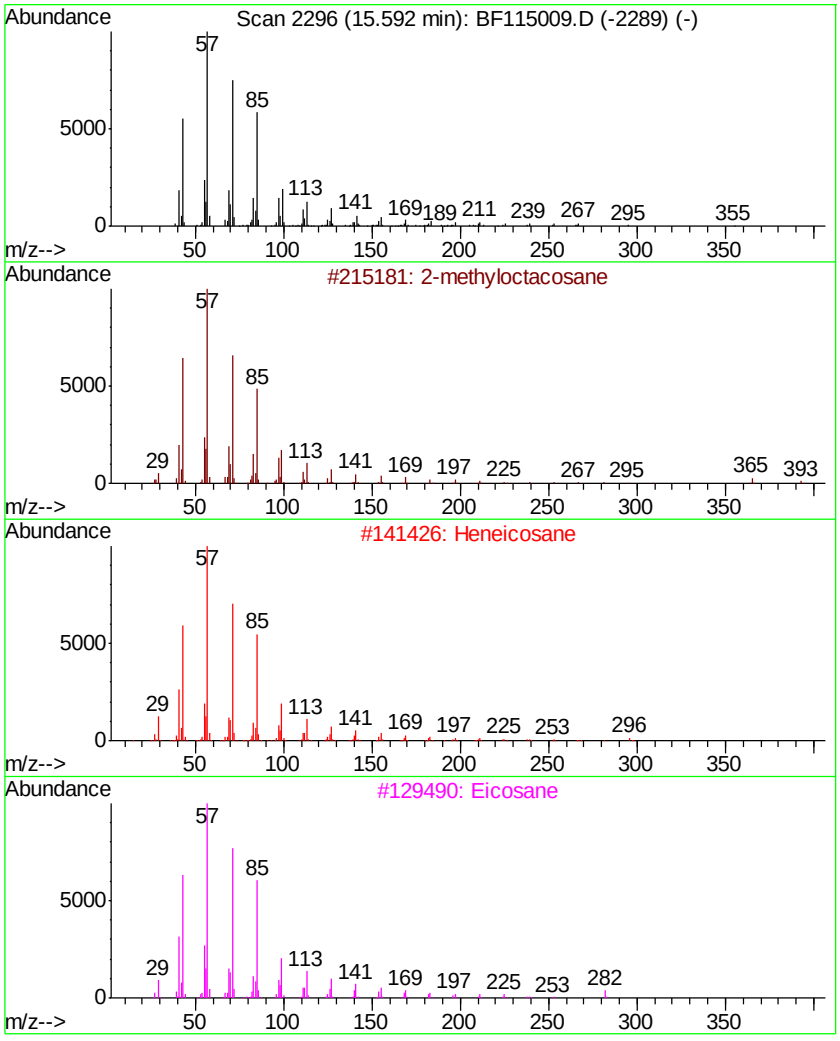
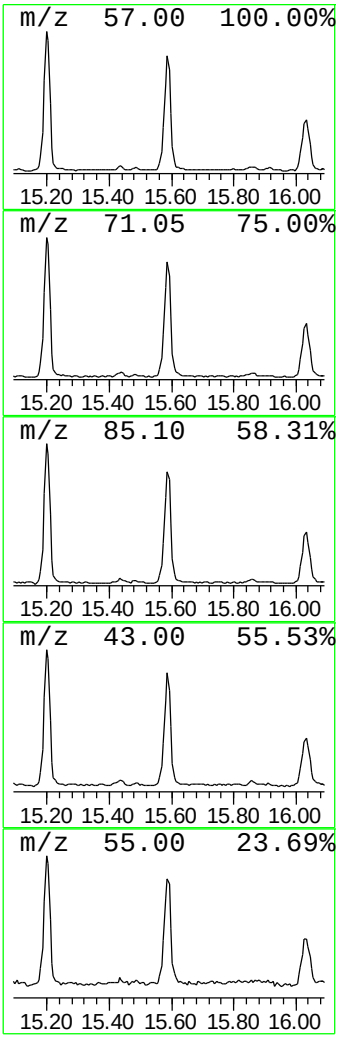
Peak Number 8 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.59	7.10 ng	585340	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Eicosane	282	C20H42	000112-95-8	91
4	Tetracosane	338	C24H50	000646-31-1	91
5	Heptadecane	240	C17H36	000629-78-7	90





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Sample : K3345-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : C-MW-11_061119

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TIC Library : C:\DATABASE\NIST11.L
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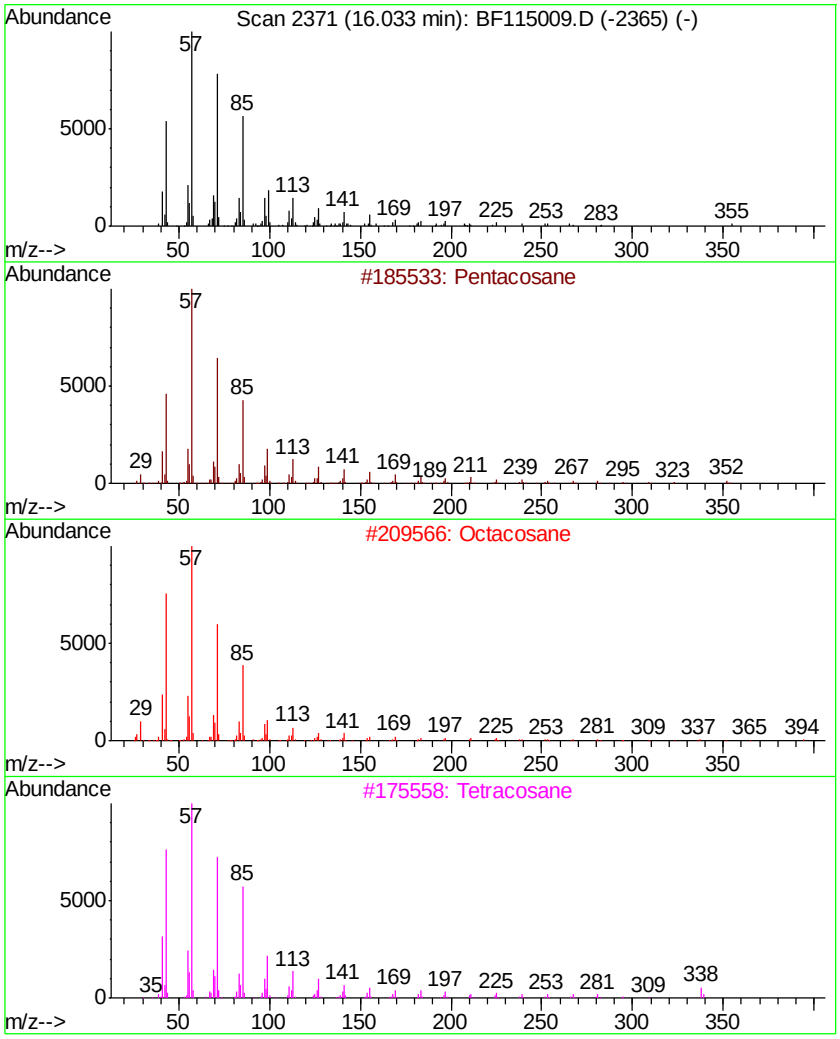
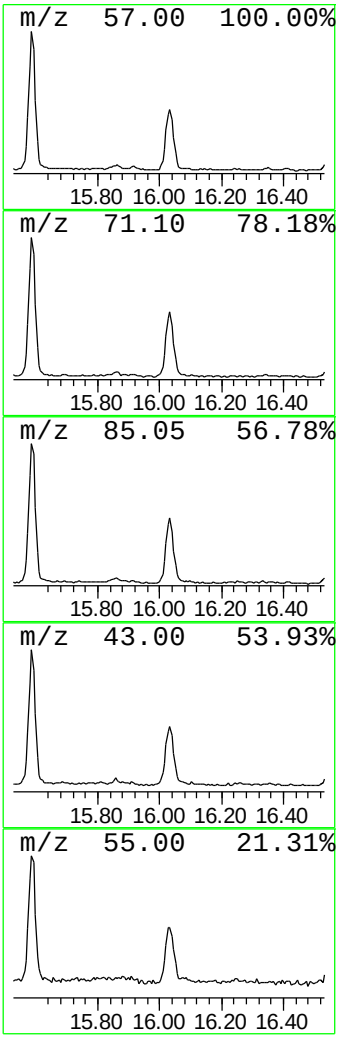
Peak Number 9 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	3.97 ng	327399	Perylene-d12	15.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Triacontane	422	C30H62	000638-68-6	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Tentatively Identified Compound (LSC) summary

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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
unknown6.42	6.42	67.7	ng	5542270	1	6.65	1636330	20.0
n-Hexadecanoic acid	11.69	2.9	ng	365621	4	11.15	2502040	20.0
Octadecanoic acid	12.47	2.0	ng	202298	5	13.77	2001740	20.0
Eicosane	14.56	3.0	ng	248524	6	15.14	1647830	20.0
2-methyloctacosane	14.86	5.9	ng	489458	6	15.14	1647830	20.0
Hexacosane	15.20	7.4	ng	608938	6	15.14	1647830	20.0
Heneicosane	15.59	7.1	ng	585340	6	15.14	1647830	20.0
Pentacosane	16.03	4.0	ng	327399	6	15.14	1647830	20.0