LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

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-BF091319.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	5.440	566	570	591	rBV	1056774	1075225	89.32%	10.791%
2	6.457	738	743	758	rBV	1077698	1191355	98.96%	11.956%
3	6.587	760	765	768	rBV	1288877	1203840	100.00%	12.081%
4	6.810	799	803	813	rBV	327958	293398	24.37%	2.944%
5	6.963	825	829	845	rBV	951968	924019	76.76%	9.273%
6	7.375	894	899	916	rBV	662919	709914	58.97%	7.124%
7	8.092	1017	1021	1035	rBV	329102	343798	28.56%	3.450%
8	9.163	1199	1203	1215	rBV	1283656	1099081	91.30%	11.030%
9	9.557	1266	1270	1280	rBV	142843	125642	10.44%	1.261%
10	9.845	1315	1319	1330	rBB	352471	326024	27.08%	3.272%
11	10.633	1449	1453	1464	rBV	504488	474014	39.38%	4.757%
12	11.327	1568	1571	1579	rBV	247540	259420	21.55%	2.603%
13	11.851	1652	1660	1667	rBV3	51943	68900	5.72%	0.691%
14	12.545	1775	1778	1785	rBV	22053	25704	2.14%	0.258%
15	12.774	1812	1817	1821	rBV	24406	27625	2.29%	0.277%
16	12.910	1836	1840	1844	rBV	826466	747023	62.05%	7.497%
17	13.480	1934	1937	1941	rBV6	13163	18684	1.55%	0.188%
18	13.816	1990	1994	2005	rBV5	55993	144094	11.97%	1.446%
19	13.974	2016	2021	2029	rBV	246093	290368	24.12%	2.914%
20	14.121	2044	2046	2049	rBV2	22701	19138	1.59%	0.192%
21	14.427	2095	2098	2102	rBV3	46886	57220	4.75%	0.574%
22	14.727	2146	2149	2153	rVB	55745	55134	4.58%	0.553%
23	14.804	2159	2162	2166	rVB	50000	61593	5.12%	0.618%
24	15.057	2202	2205	2211	rVB	82543	88284	7.33%	0.886%
25	15.427	2264	2268	2275	rVB2	198807	257911	21.42%	2.588%
26	15.851	2336	2340	2344	rVB	57206	77125	6.41%	0.774%

Sum of corrected areas: 9964533

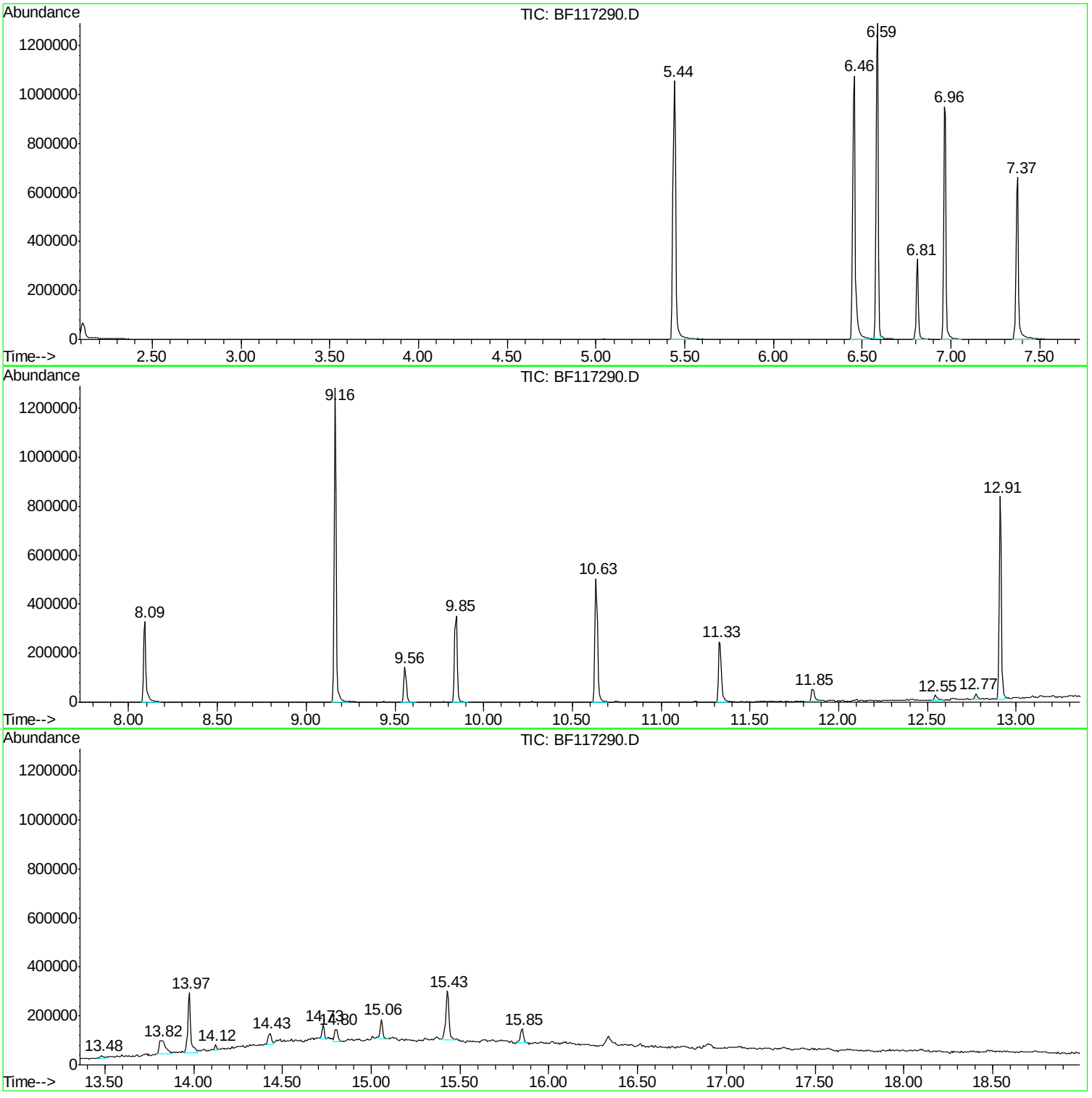
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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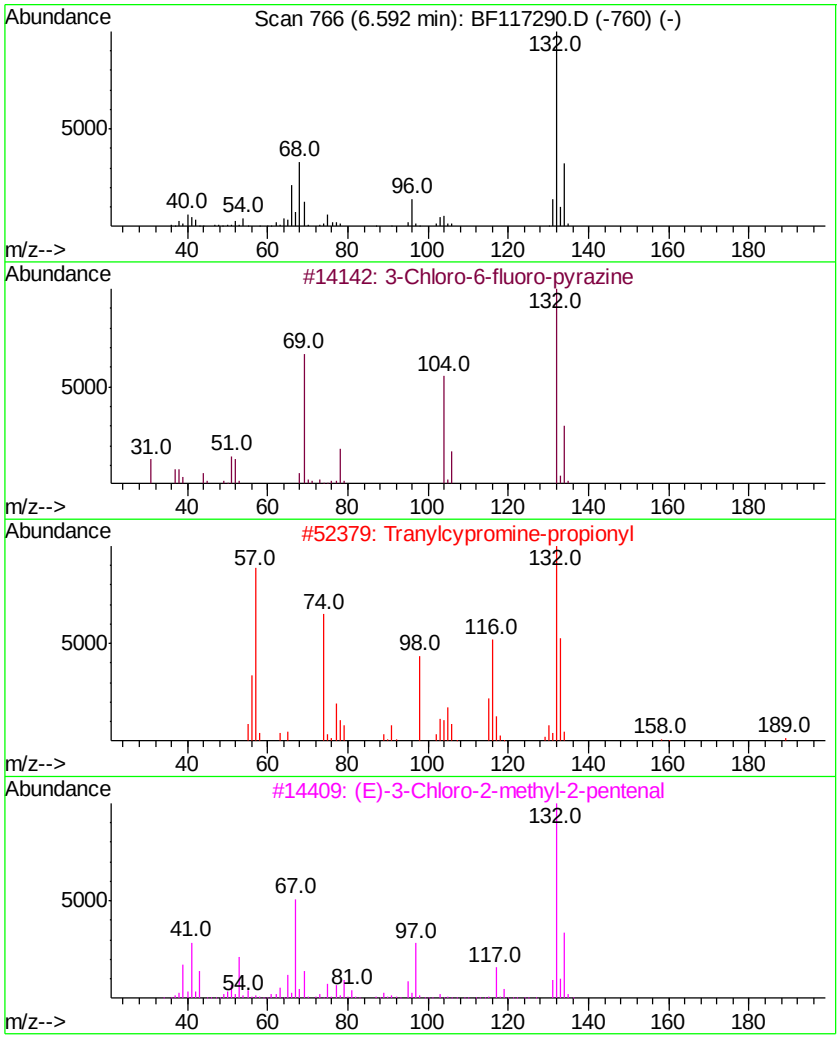
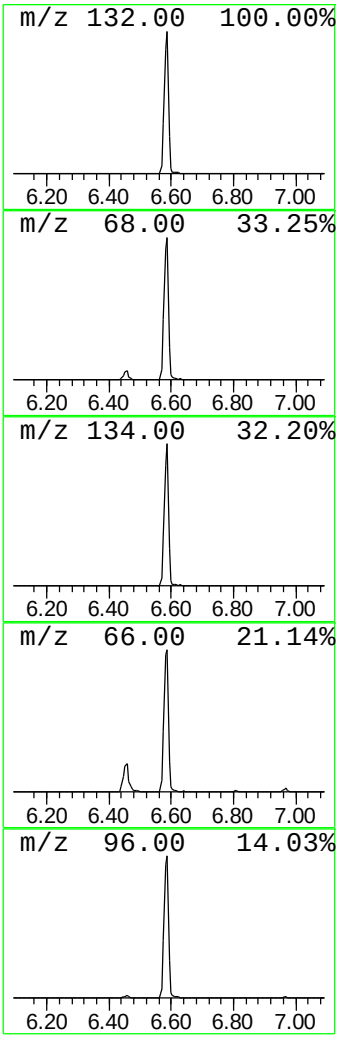
Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	82.06 ng	1203840	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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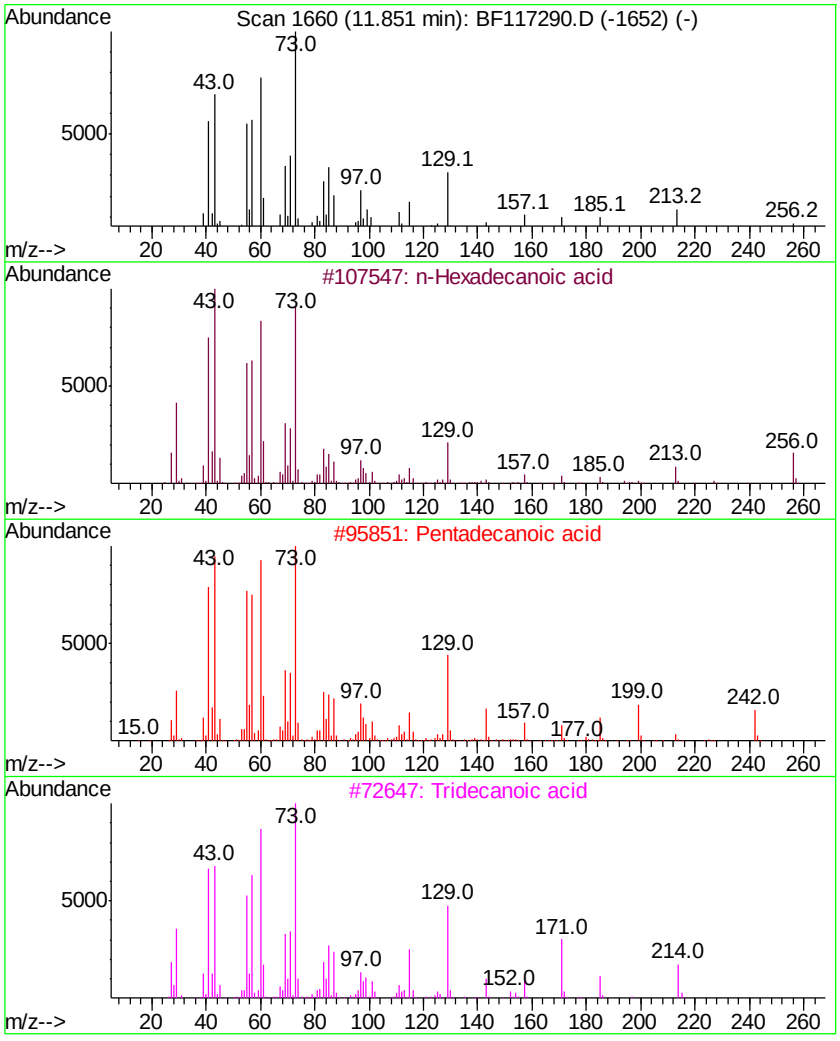
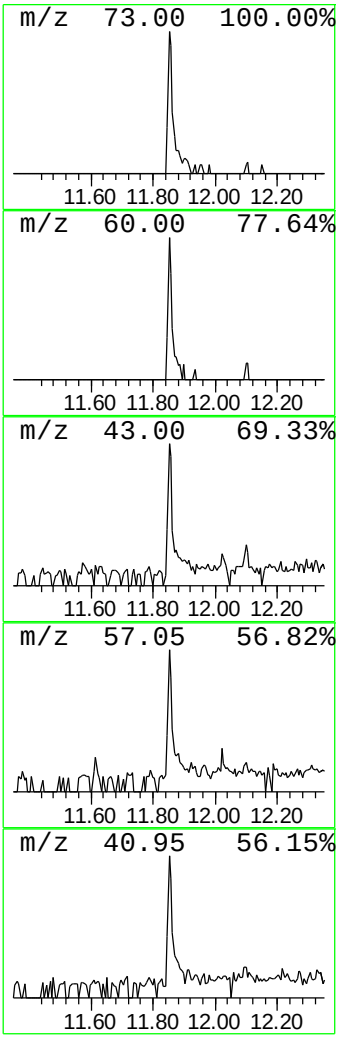
Peak Number 3 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	5.31 ng	68900	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3	Tridecanoic acid	214	C13H26O2	000638-53-9	53
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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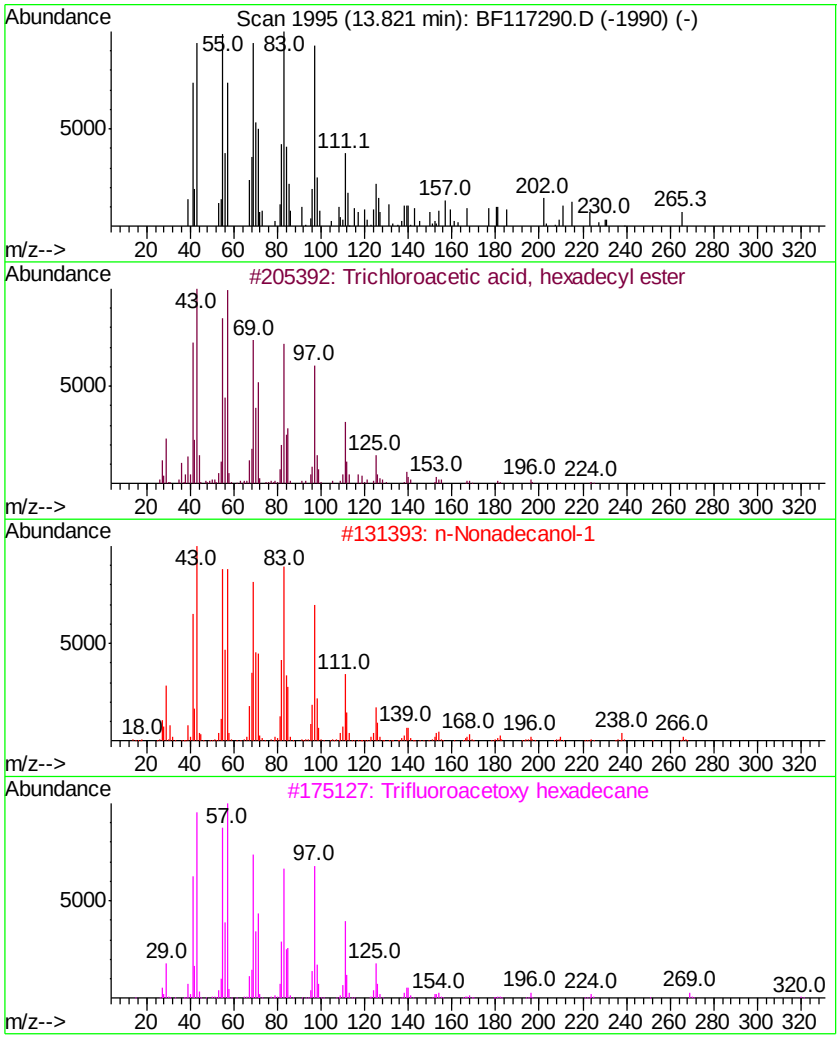
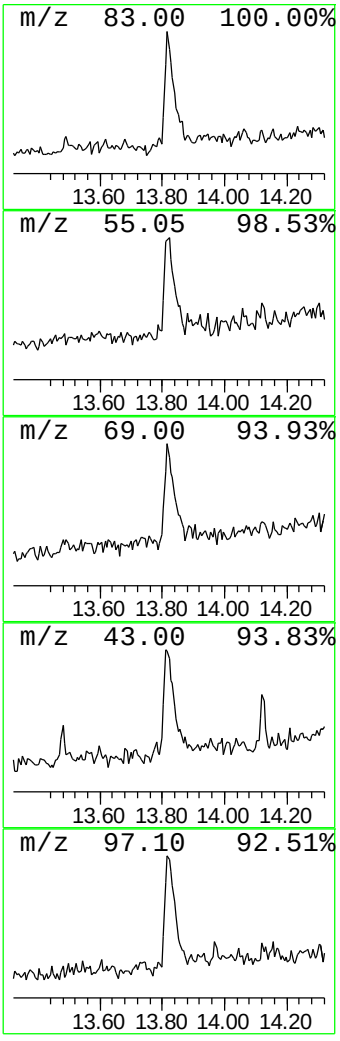
Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	9.92 ng	144094	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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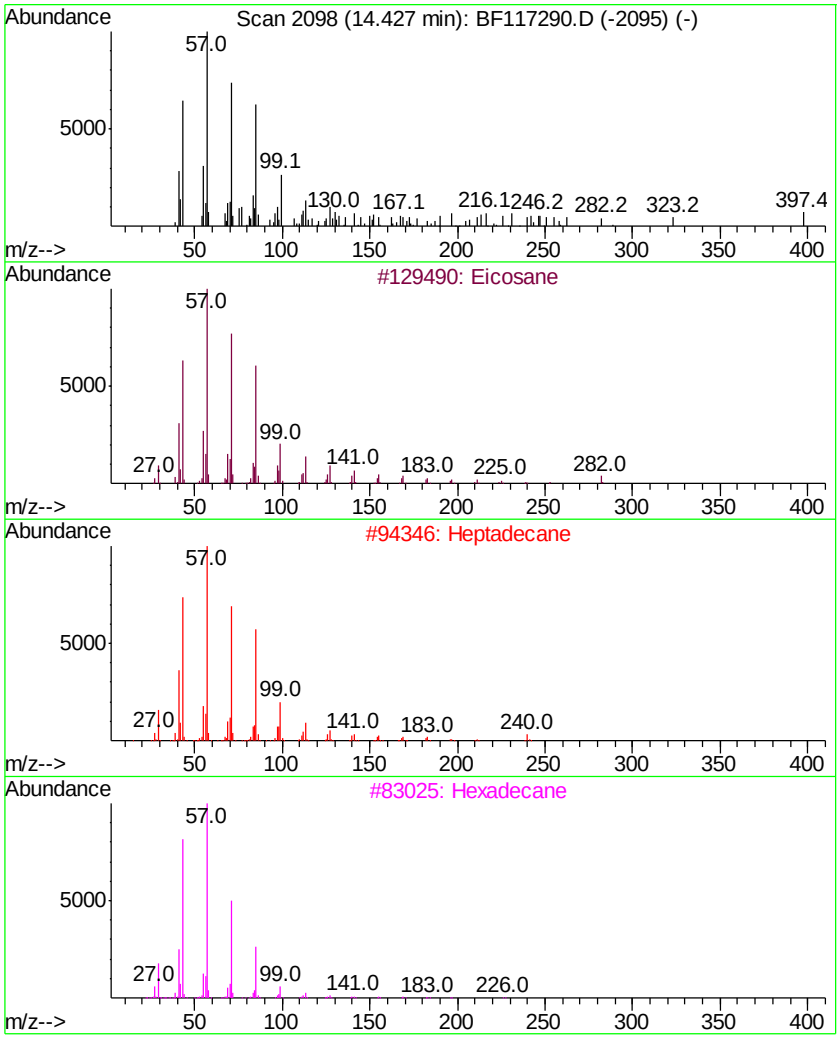
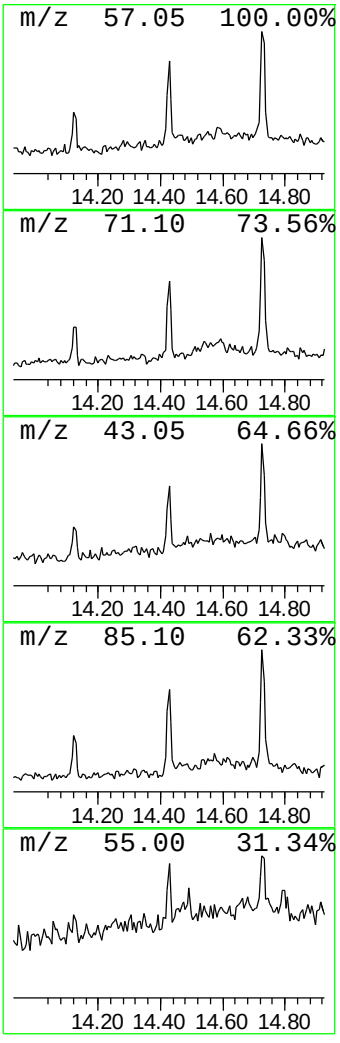
Peak Number 5 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.43	3.94 ng	57220	Chrysene-d12	13.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Heptadecane	240	C17H36	000629-78-7	93
3	Hexadecane	226	C16H34	000544-76-3	93
4	Heneicosane	296	C21H44	000629-94-7	81
5	Octacosane	394	C28H58	000630-02-4	74





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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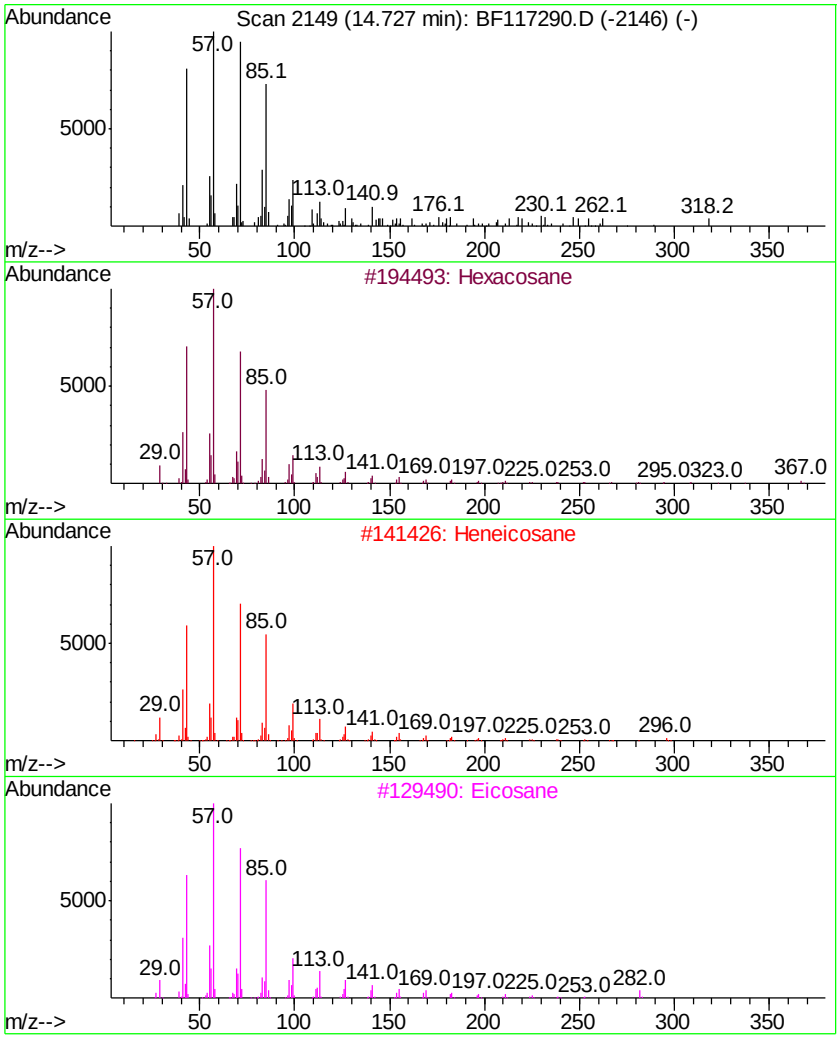
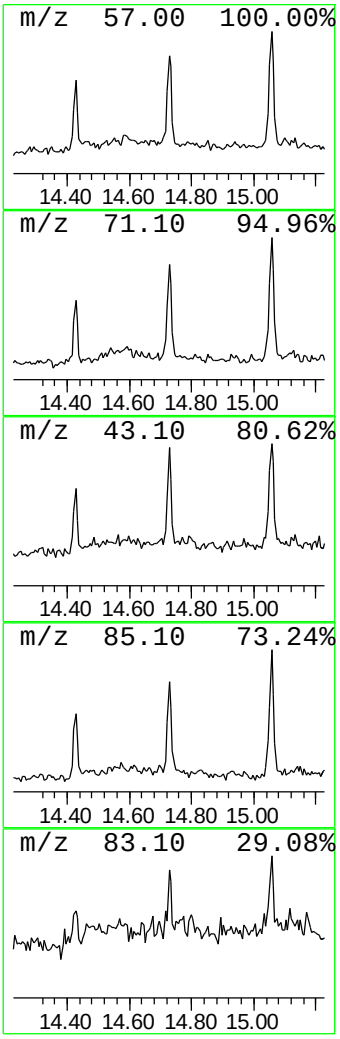
Peak Number 6 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	4.28 ng	55134	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	72
2	Heneicosane	296	C21H44	000629-94-7	72
3	Eicosane	282	C20H42	000112-95-8	72
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
5	Dodecane, 4-methyl-	184	C13H28	006117-97-1	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

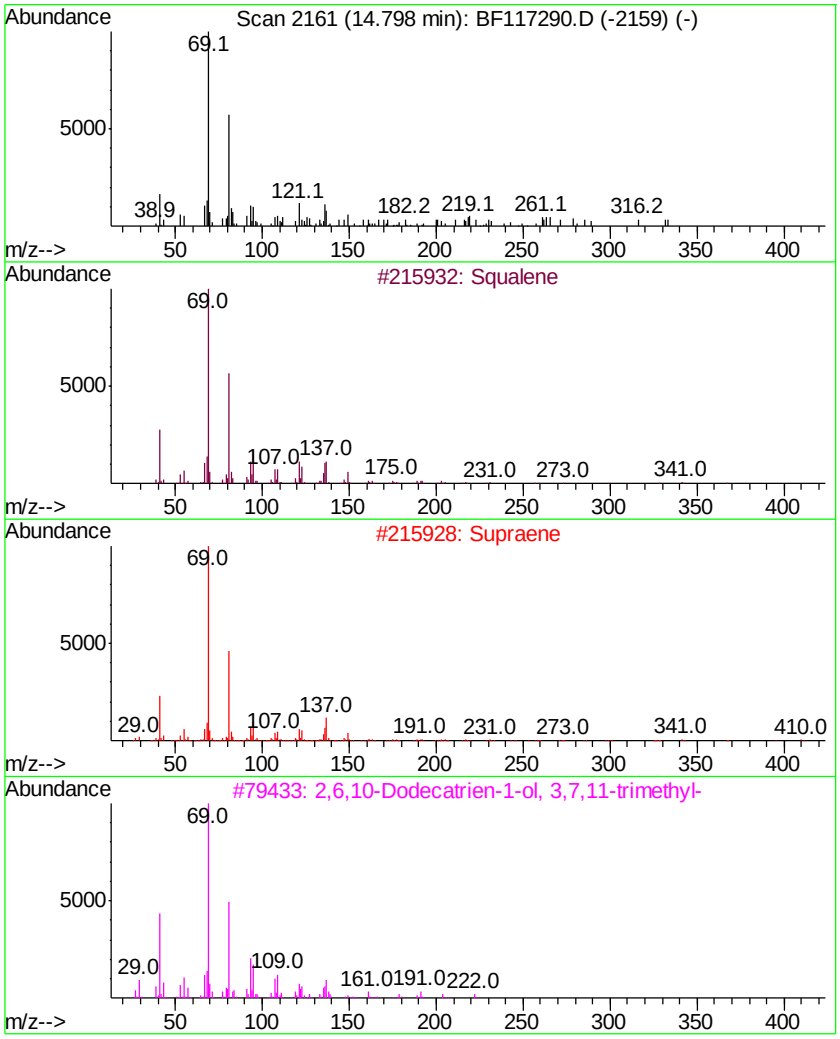
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

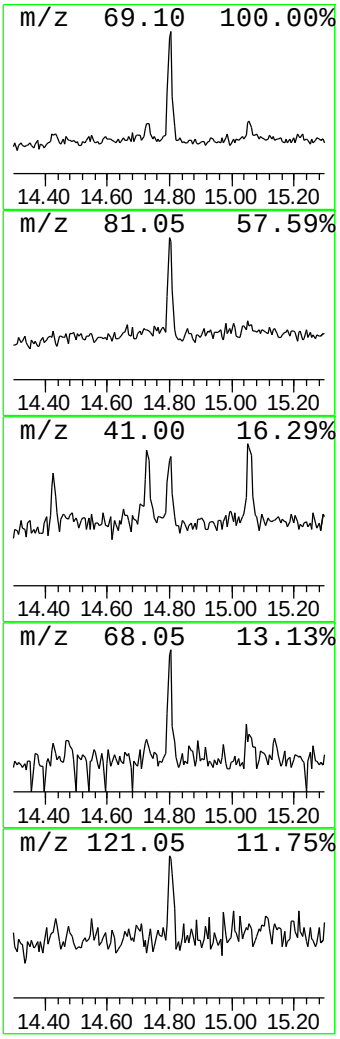
****

Peak Number 7 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	4.78 ng	61593	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	72
2	Supraene	410	C30H50	007683-64-9	72
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	68
4	trans-Farnesol	222	C15H26O	000106-28-5	59
5	6,11-Dimethyl-2,6,10-dodecatrien...	208	C14H24O	1000196-53-3	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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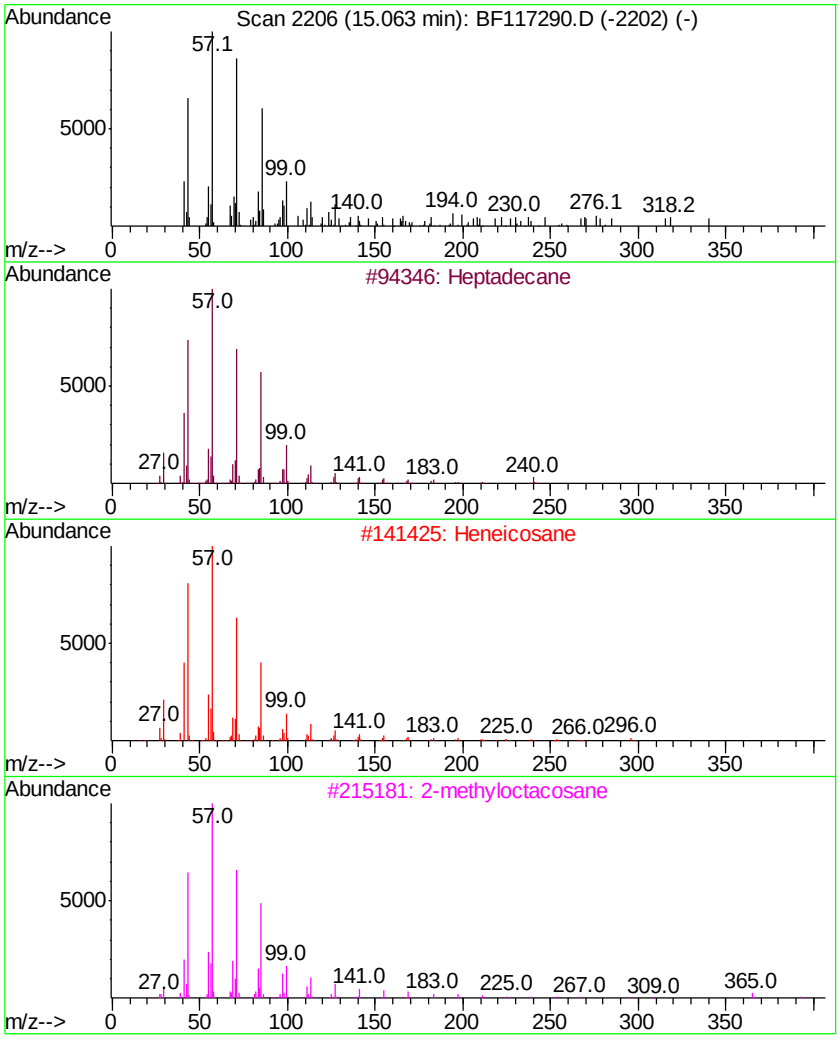
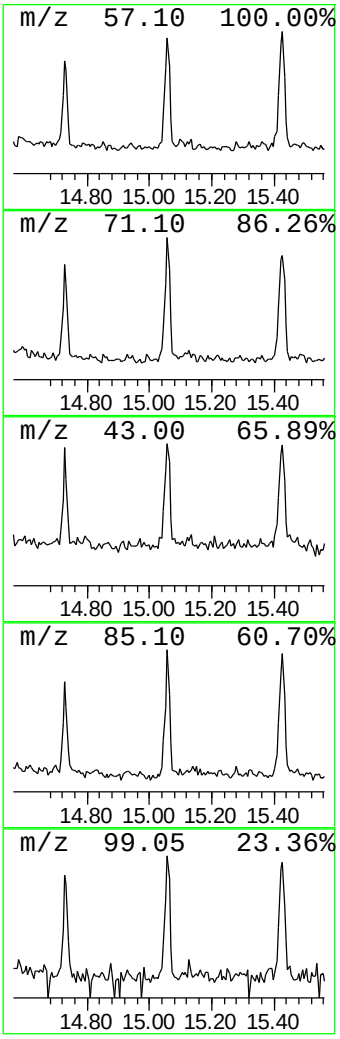
Peak Number 8 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	6.85 ng	88284	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	74
2	Heneicosane	296	C21H44	000629-94-7	74
3	2-methyloctacosane	408	C29H60	1000376-72-8	74
4	Octacosane	394	C28H58	000630-02-4	72
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF100119\
Data File : BF117290.D
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Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

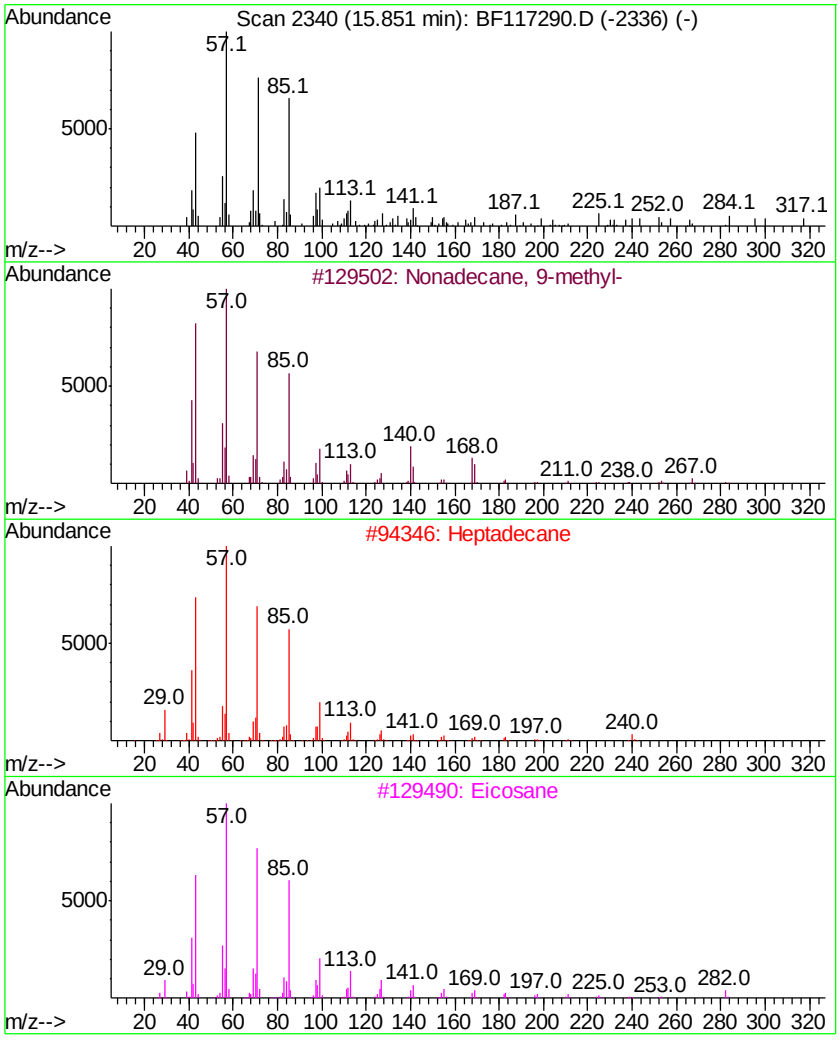
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

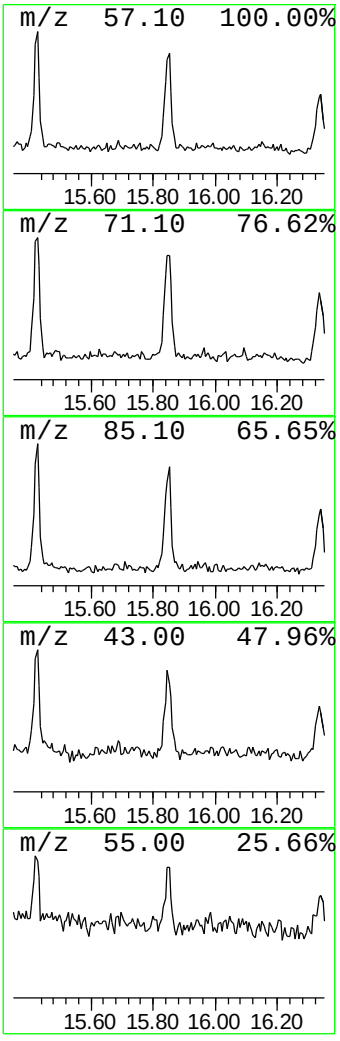
****

Peak Number 9 Nonadecane, 9-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.85	5.98 ng	77125	Perylene-d12	15.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Heptadecane	240	C17H36	000629-78-7	93
3	Eicosane	282	C20H42	000112-95-8	90
4	Octacosane	394	C28H58	000630-02-4	74
5	Heneicosane	296	C21H44	000629-94-7	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF100119\
Data File : BF117290.D
Acq On : 1 Oct 2019 21:23
Operator : JU
Sample : K4946-06
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-3_(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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
unknown6.59	6.59	82.1	ng	1203840	1	6.81	293398	20.0
n-Hexadecanoic acid	11.85	5.3	ng	68900	4	11.33	259420	20.0
Trichloroacetic a...	13.82	9.9	ng	144094	5	13.97	290368	20.0
Eicosane	14.43	3.9	ng	57220	5	13.97	290368	20.0
Hexacosane	14.73	4.3	ng	55134	6	15.43	257911	20.0
Squalene	14.80	4.8	ng	61593	6	15.43	257911	20.0
Heptadecane	15.06	6.8	ng	88284	6	15.43	257911	20.0
Nonadecane, 9-met...	15.85	6.0	ng	77125	6	15.43	257911	20.0