LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
Data File : BF116071.D
Acq On : 8 Aug 2019 16:13
Operator : HP/JU
Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

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-BF073019.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	5.457	570	573	597	rBV	1462636	1748871	34.37%	5.271%
2	6.469	742	745	765	rBV	1317836	1394754	27.41%	4.204%
3	6.610	765	769	772	rBV	3255552	2897969	56.96%	8.734%
4	6.834	804	807	817	rBV	815576	796934	15.66%	2.402%
5	6.992	830	834	846	rBV	2708910	2573740	50.58%	7.757%
6	7.398	899	903	917	rBV	2093715	2209940	43.43%	6.660%
7	8.116	1022	1025	1045	rBV	1030769	1024846	20.14%	3.089%
8	9.192	1203	1208	1211	rBV	4191704	3897457	76.60%	11.746%
9	9.586	1271	1275	1285	rBV	364717	401517	7.89%	1.210%
10	9.869	1319	1323	1337	rVB	1456724	1269873	24.96%	3.827%
11	10.280	1390	1393	1399	rVB	97741	96613	1.90%	0.291%
12	10.663	1453	1458	1474	rBV	2473864	2624634	51.58%	7.910%
13	11.357	1572	1576	1584	rBV	1377613	1357730	26.69%	4.092%
14	11.733	1635	1640	1643	rVB2	73656	63429	1.25%	0.191%
15	11.880	1661	1665	1668	rBV	133615	149684	2.94%	0.451%
16	12.663	1795	1798	1812	rBV	106957	188509	3.70%	0.568%
17	12.945	1840	1846	1849	rBV	4641165	5087987	100.00%	15.334%
18	13.833	1993	1997	2015	rBV	236604	472646	9.29%	1.424%
19	13.963	2015	2019	2021	rVV	56723	52739	1.04%	0.159%
20	13.998	2021	2025	2039	rVB	1310769	1389808	27.32%	4.189%
21	14.145	2047	2050	2054	rBV	81605	76740	1.51%	0.231%
22	14.451	2098	2102	2106	rBV	200343	194036	3.81%	0.585%
23	14.751	2148	2153	2161	rBV	336850	335369	6.59%	1.011%
24	14.827	2162	2166	2172	rVB	306880	291501	5.73%	0.879%
25	15.086	2205	2210	2218	rVB	362626	412776	8.11%	1.244%
26	15.457	2268	2273	2288	rBV	1064973	1565399	30.77%	4.718%
27	15.880	2340	2345	2352	rBV	212070	331034	6.51%	0.998%
28	16.380	2424	2430	2443	rVB	100260	203795	4.01%	0.614%
29	16.956	2523	2528	2537	rVB2	31698	69839	1.37%	0.210%

Sum of corrected areas: 33180169

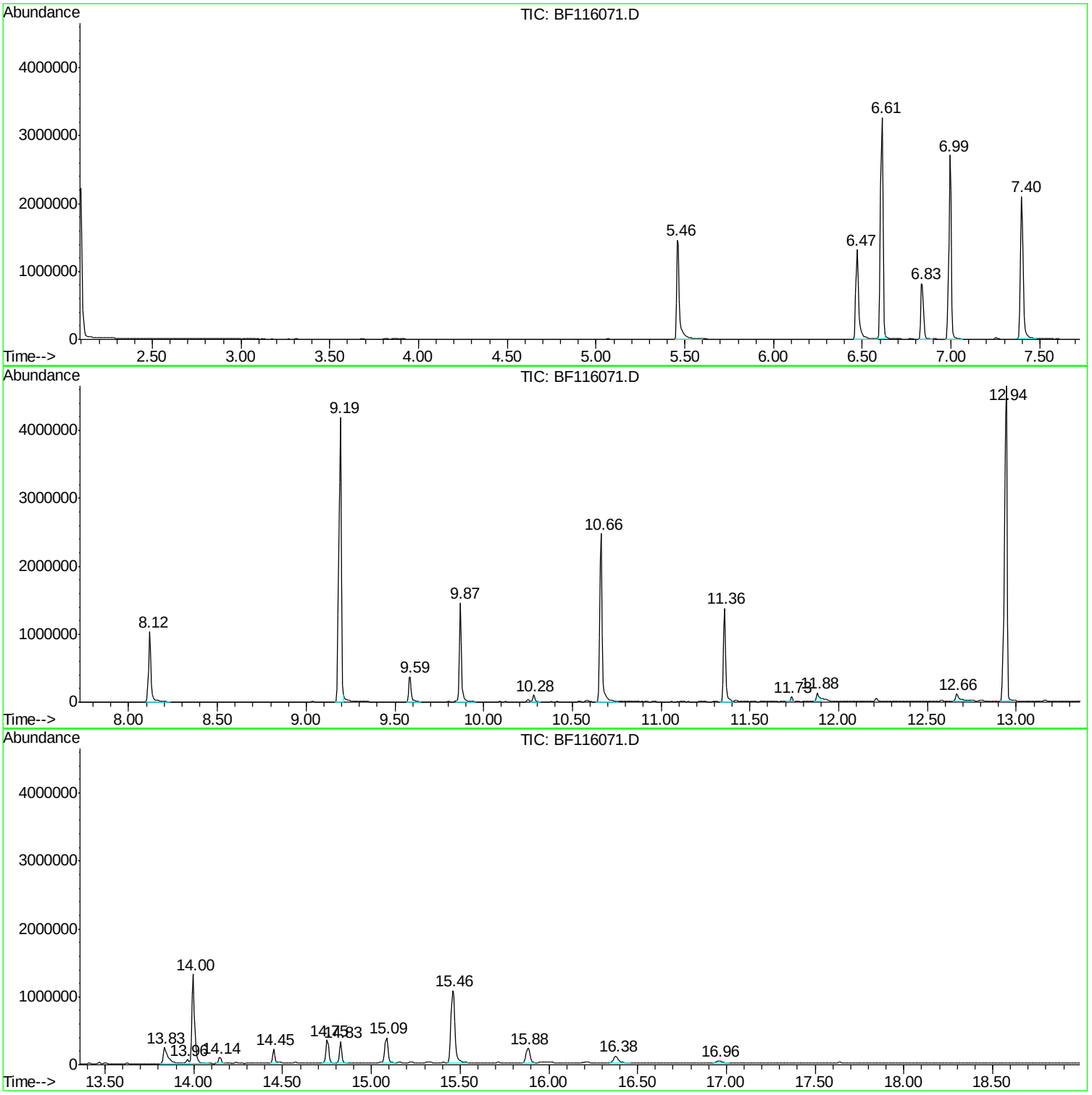
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
Data File : BF116071.D
Acq On : 8 Aug 2019 16:13
Operator : HP/JU
Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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Data File : BF116071.D
Acq On : 8 Aug 2019 16:13
Operator : HP/JU
Sample : K4148-04
Misc :
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Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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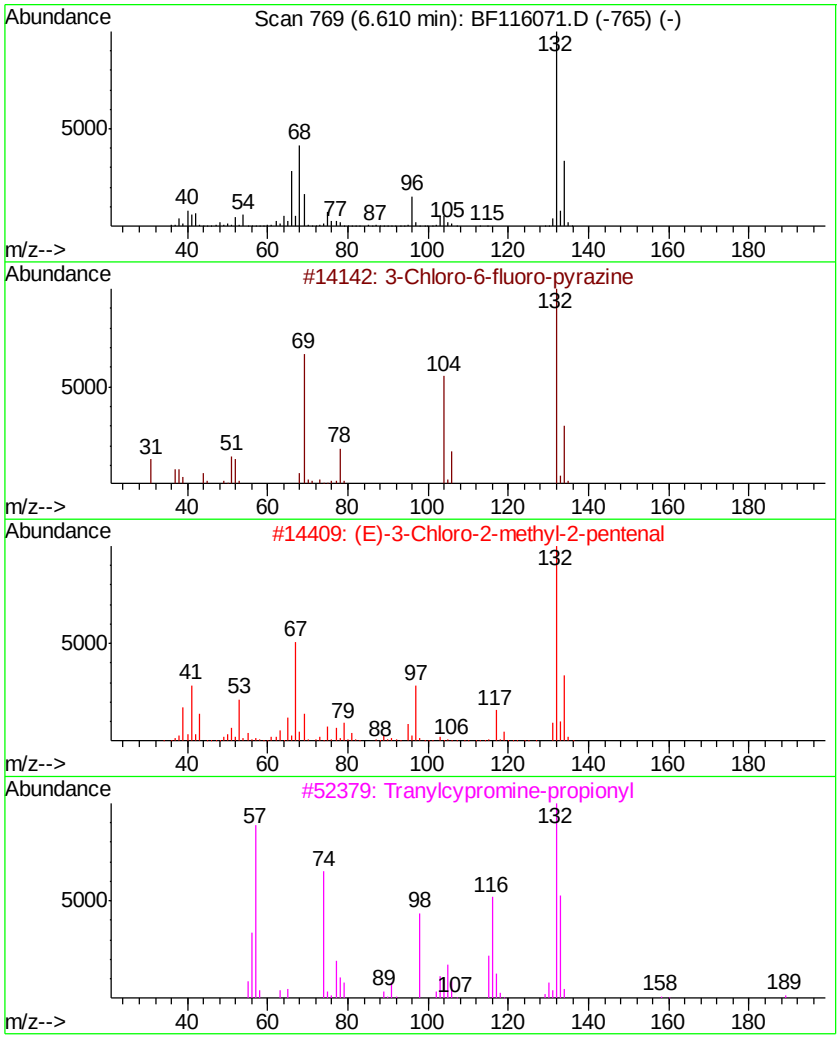
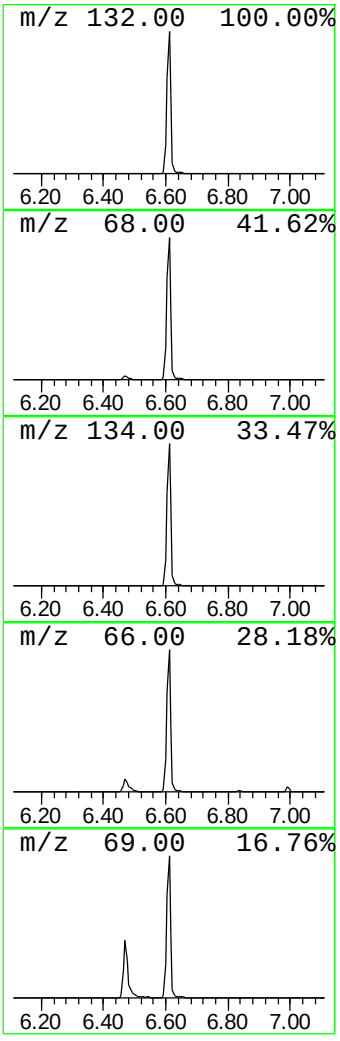
Peak Number 1 unknown6.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.61	72.73 ng	2897970	1,4-Dichlorobenzene-d4	6.84

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





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Data File : BF116071.D
Acq On : 8 Aug 2019 16:13
Operator : HP/JU
Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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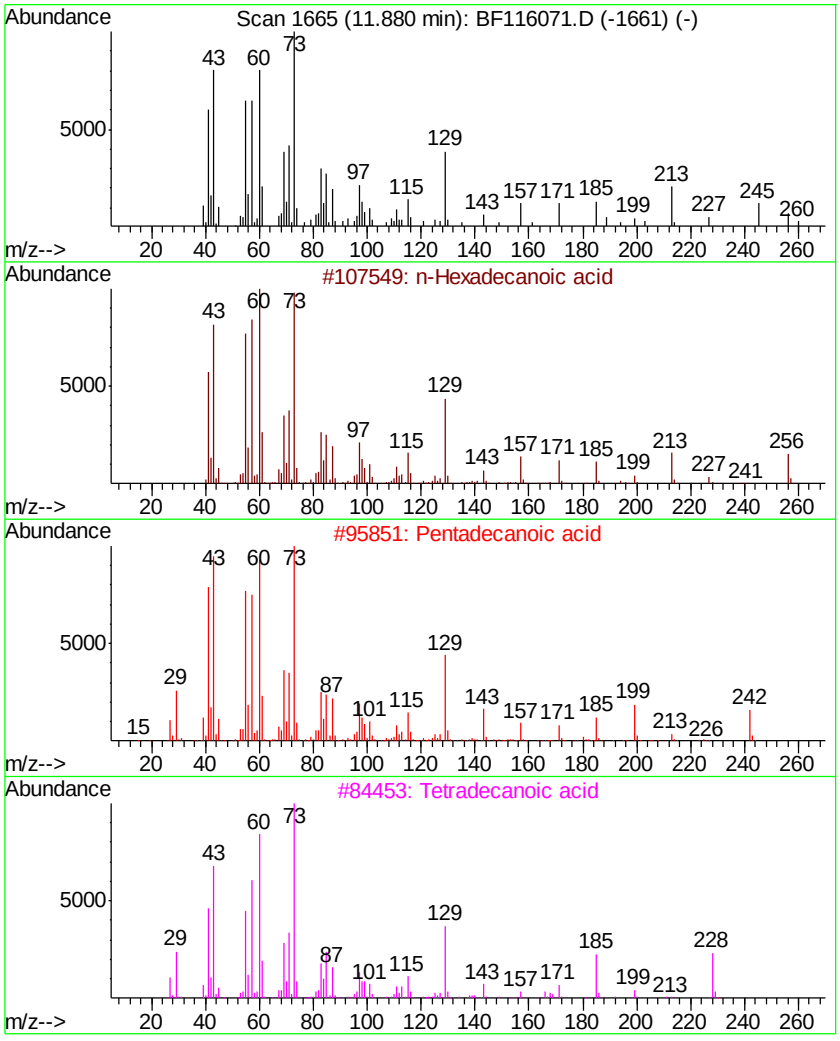
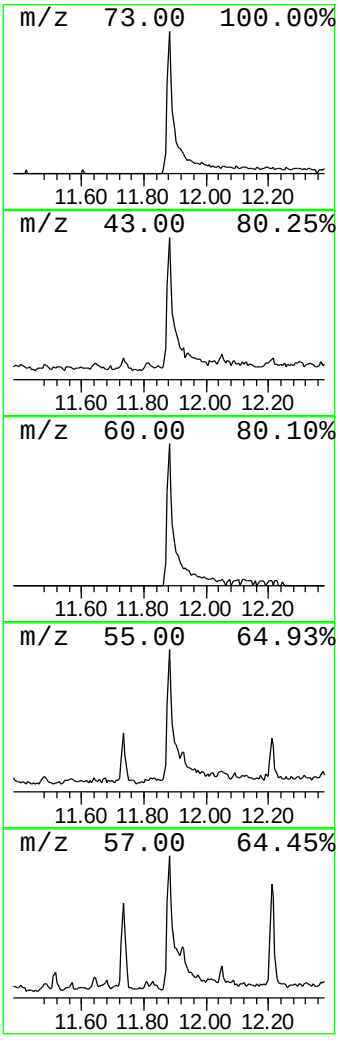
Peak Number 3 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	2.20 ng	149684	Phenanthrene-d10	11.36

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
Data File : BF116071.D
Acq On : 8 Aug 2019 16:13
Operator : HP/JU
Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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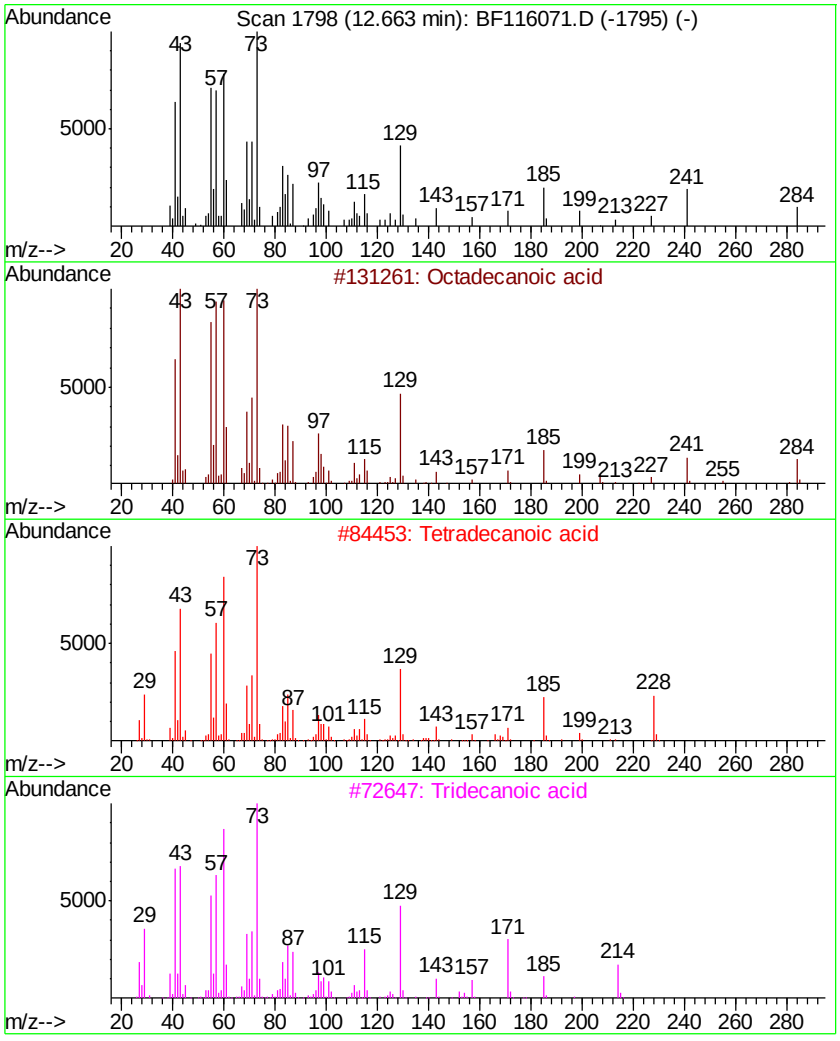
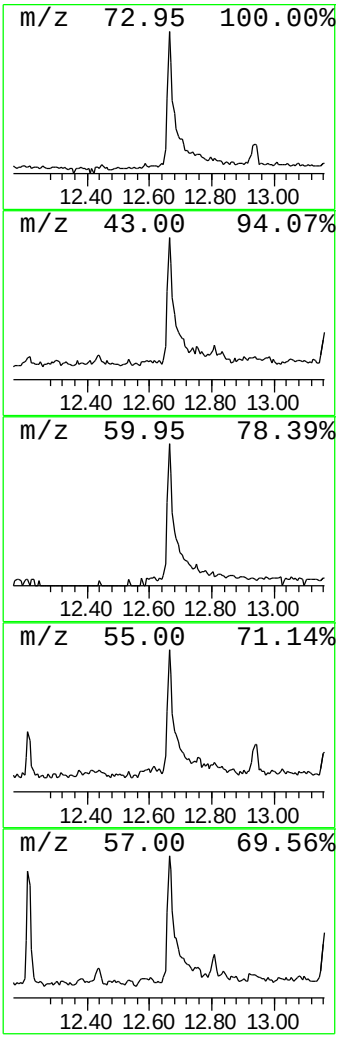
Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.66	2.78 ng	188509	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	80
4	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
Data File : BF116071.D
Acq On : 8 Aug 2019 16:13
Operator : HP/JU
Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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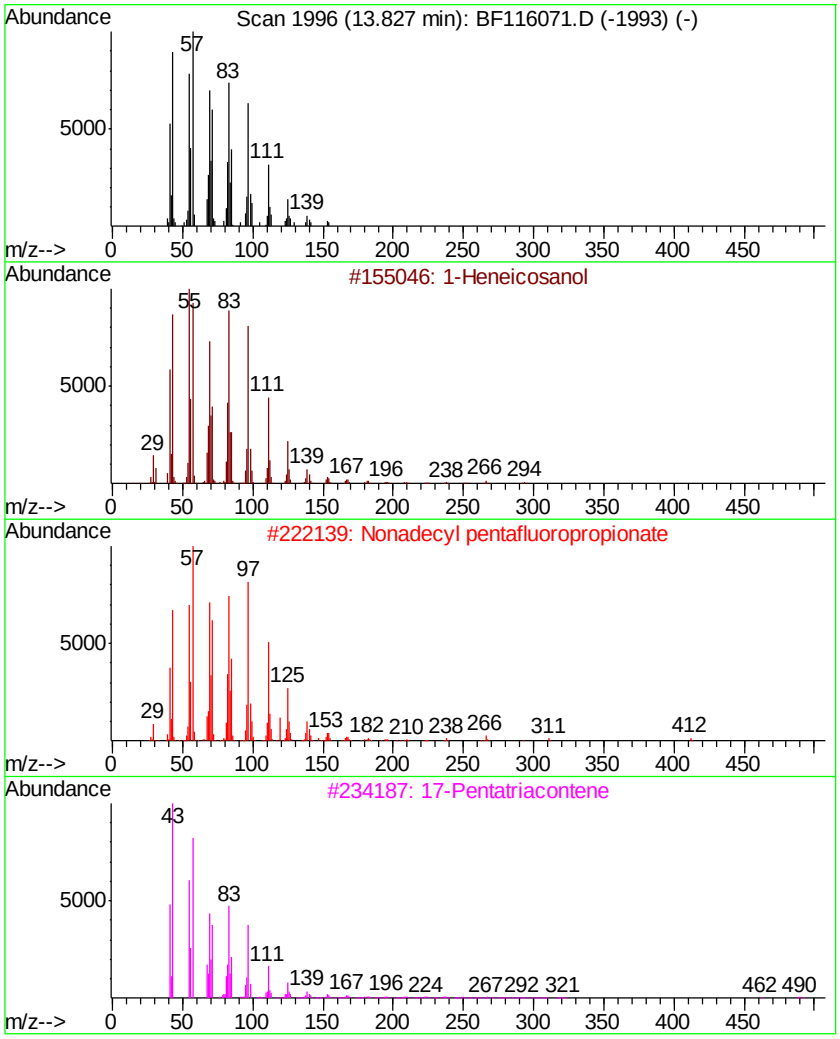
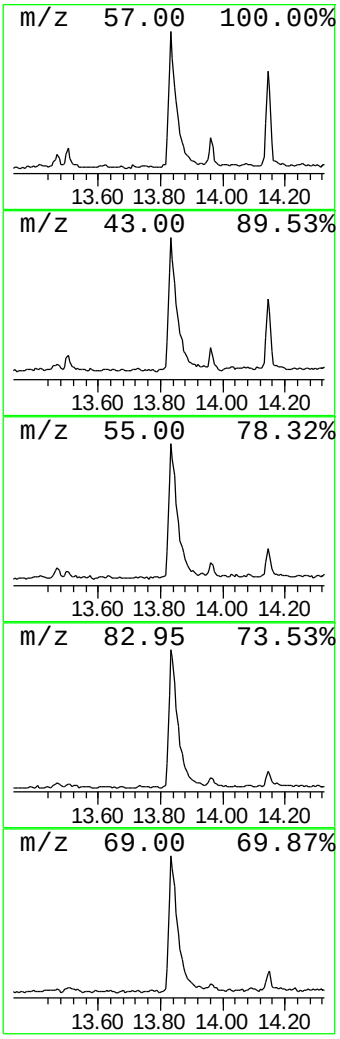
Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	6.80 ng	472646	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF080819\
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Operator : HP/JU
Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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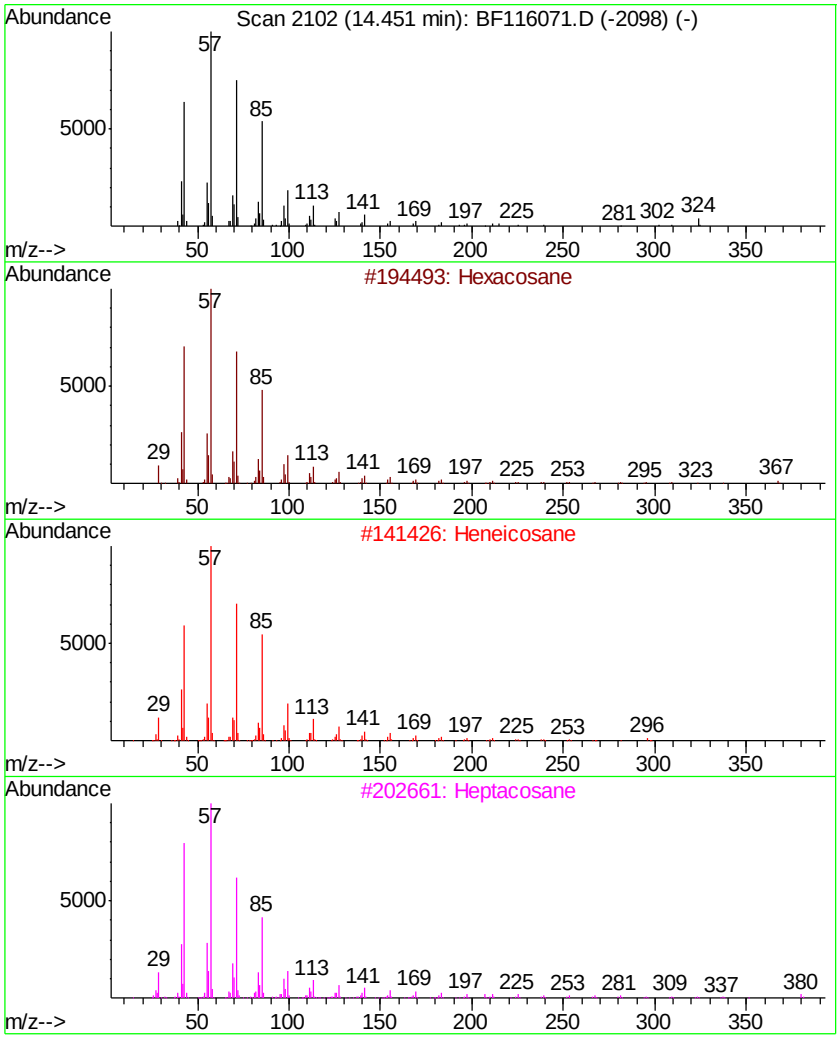
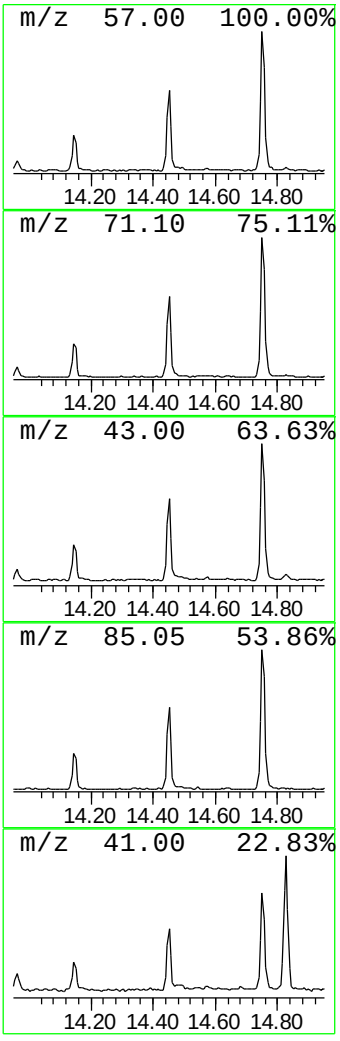
Peak Number 6 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	2.79 ng	194036	Chrysene-d12	14.00

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	Heptacosane	380	C27H56	000593-49-7	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





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Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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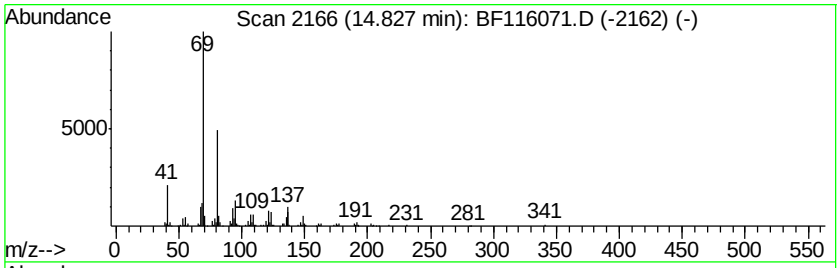
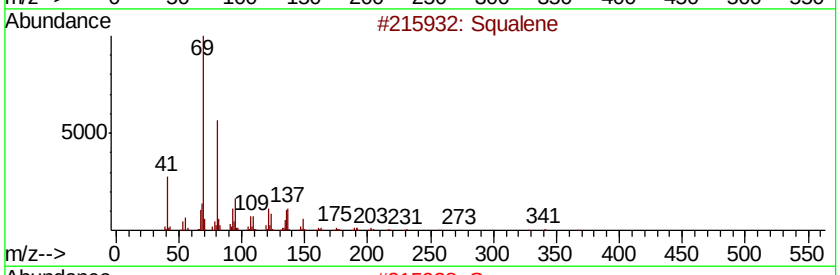
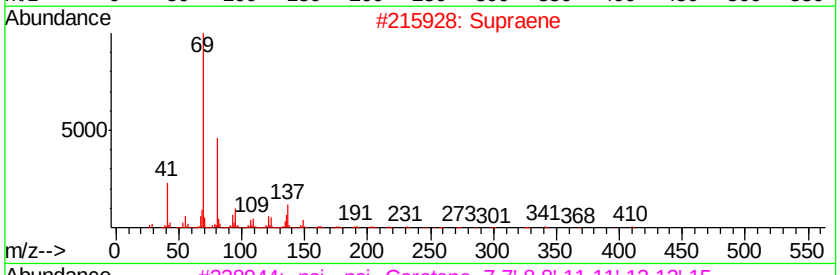
Peak Number 8 Squalene Concentration Rank 7

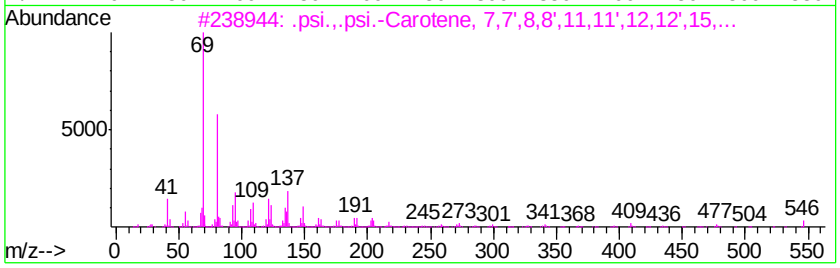
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.72 ng	291501	Perylene-d12	15.46

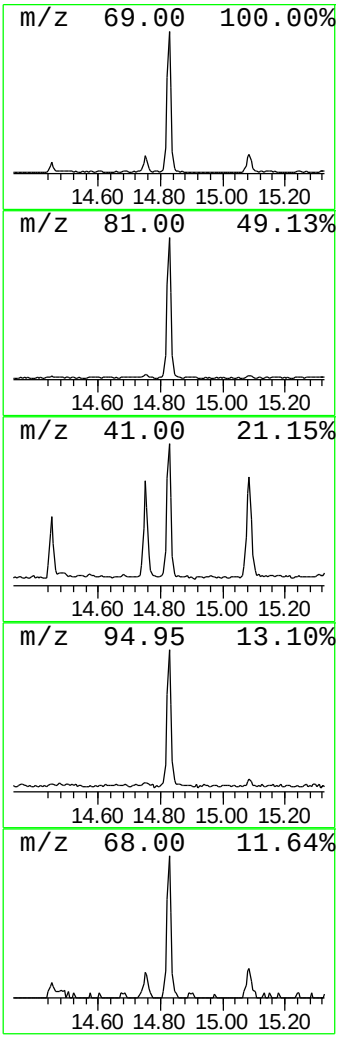
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	52











Library Search Compound Report

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Data File : BF116071.D
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Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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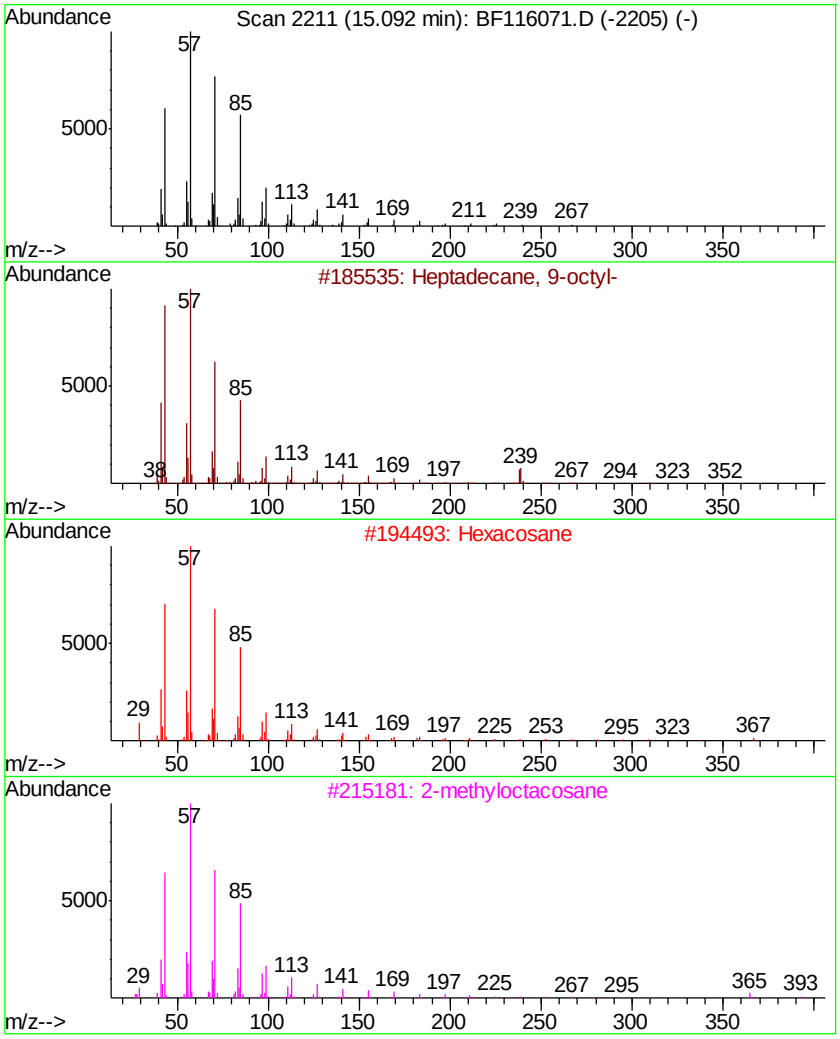
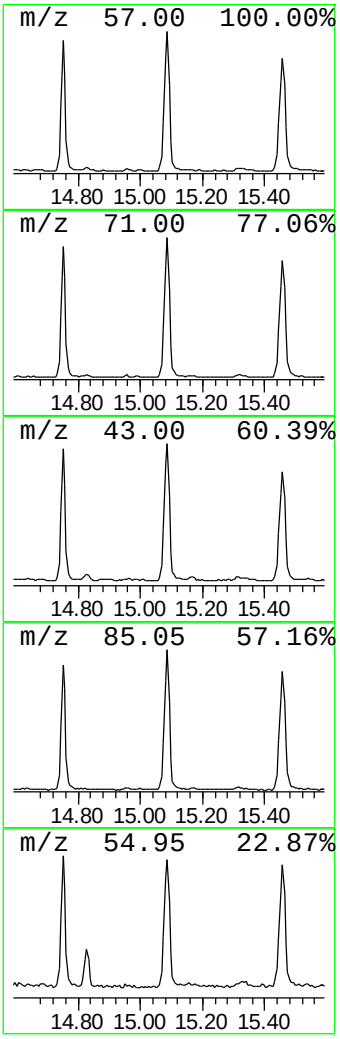
Peak Number 9 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	5.27 ng	412776	Perylene-d12	15.46

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





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Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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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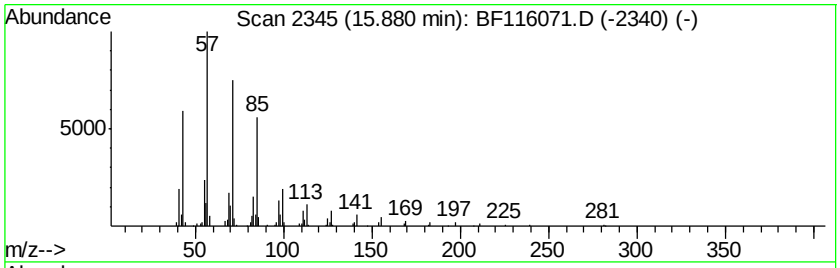
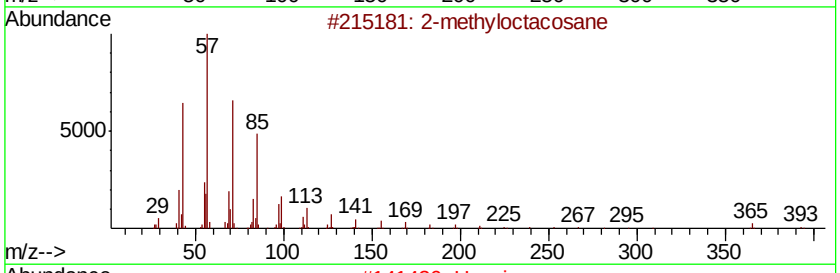
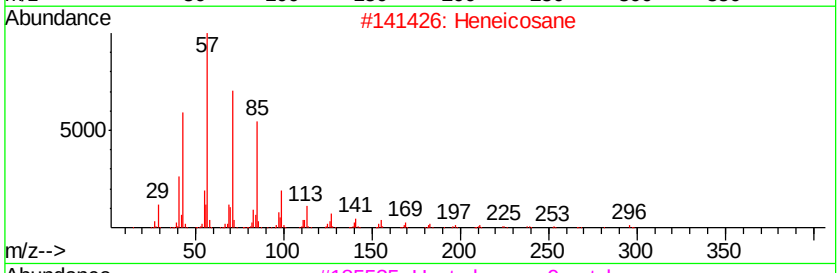
Peak Number 10 2-methyloctacosane Concentration Rank 6

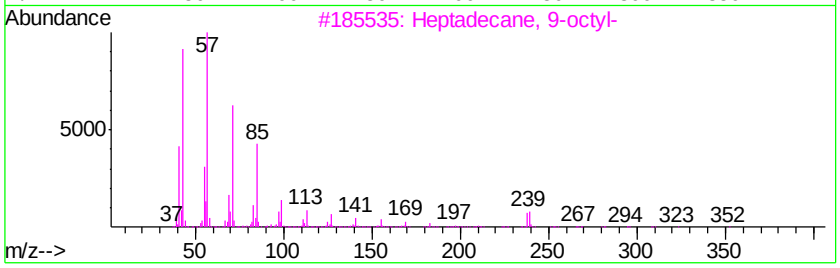
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	4.23 ng	331034	Perylene-d12	15.46

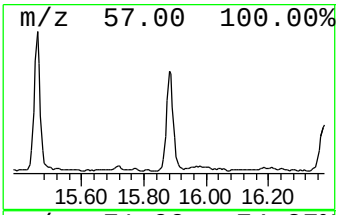
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	90
5	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90

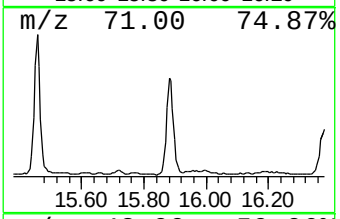


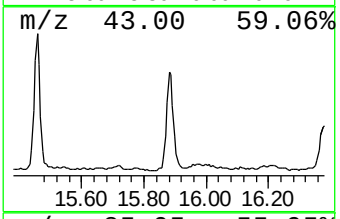


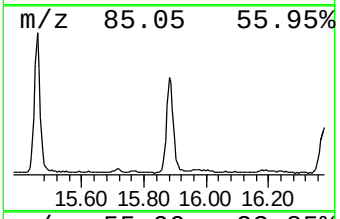


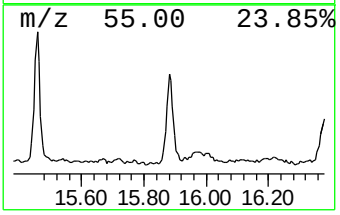












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF080819\
Data File : BF116071.D
Acq On : 8 Aug 2019 16:13
Operator : HP/JU
Sample : K4148-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMP-BH-2-ELU-20190611

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF073019.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
unknown6.61	6.61	72.7	ng	2897970	1	6.84	796934	20.0
n-Hexadecanoic acid	11.88	2.2	ng	149684	4	11.36	1357730	20.0
Octadecanoic acid	12.66	2.8	ng	188509	4	11.36	1357730	20.0
1-Heneicosanol	13.83	6.8	ng	472646	5	14.00	1389810	20.0
Hexacosane	14.45	2.8	ng	194036	5	14.00	1389810	20.0
Squalene	14.83	3.7	ng	291501	6	15.46	1565400	20.0
Heptadecane, 9-oc...	15.09	5.3	ng	412776	6	15.46	1565400	20.0
2-methyloctacosane	15.88	4.2	ng	331034	6	15.46	1565400	20.0