LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

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-BF083019.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	5.463	570	574	578	rBV	1557278	1506671	78.05%	8.412%
2	6.481	742	747	756	rBV	1774047	1715248	88.86%	9.576%
3	6.616	766	770	773	rBV	1968928	1700054	88.07%	9.492%
4	6.845	805	809	812	rBV	721452	552671	28.63%	3.086%
5	7.004	832	836	839	rBV	1558364	1277807	66.19%	7.134%
6	7.404	899	904	907	rBV	1203275	1008848	52.26%	5.633%
7	8.128	1023	1027	1030	rBV	913481	737706	38.22%	4.119%
8	9.198	1205	1209	1212	rBV	2240804	1930369	100.00%	10.777%
9	9.586	1272	1275	1279	rBV	164569	130990	6.79%	0.731%
10	9.881	1321	1325	1328	rBV	1119479	879197	45.55%	4.909%
11	10.669	1454	1459	1462	rBV	1097594	1056496	54.73%	5.899%
12	11.363	1573	1577	1580	rBV	1041709	855874	44.34%	4.778%
13	11.886	1662	1666	1669	rBV	73127	73796	3.82%	0.412%
14	12.569	1779	1782	1787	rBV	63368	65322	3.38%	0.365%
15	12.669	1795	1799	1801	rBV4	24083	24831	1.29%	0.139%
16	12.798	1816	1821	1823	rBV	58862	58038	3.01%	0.324%
17	12.945	1841	1846	1849	rBV	1918132	1718134	89.01%	9.593%
18	13.174	1883	1885	1893	rVB6	20232	22989	1.19%	0.128%
19	13.516	1940	1943	1945	rVB	29558	21290	1.10%	0.119%
20	13.833	1993	1997	2008	rBV2	234709	312938	16.21%	1.747%
21	13.998	2018	2025	2028	rBV	807017	813083	42.12%	4.540%
22	14.157	2049	2052	2057	rBV	55152	47838	2.48%	0.267%
23	14.463	2101	2104	2109	rVB2	76202	81646	4.23%	0.456%
24	14.763	2152	2155	2160	rBV	84258	81431	4.22%	0.455%
25	15.027	2197	2200	2203	rBV2	25165	34066	1.76%	0.190%
26	15.098	2209	2212	2218	rBV	105565	128771	6.67%	0.719%
27	15.386	2258	2261	2264	rBV2	19424	24749	1.28%	0.138%
28	15.457	2267	2273	2282	rVB	488649	747027	38.70%	4.171%
29	15.910	2345	2350	2354	rBV2	80542	121164	6.28%	0.676%
30	15.957	2355	2358	2364	rBV8	23915	47989	2.49%	0.268%
31	16.404	2430	2434	2441	rVB	54513	91997	4.77%	0.514%
32	16.992	2531	2534	2541	rVB7	22727	42095	2.18%	0.235%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

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-BF083019.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 17911125

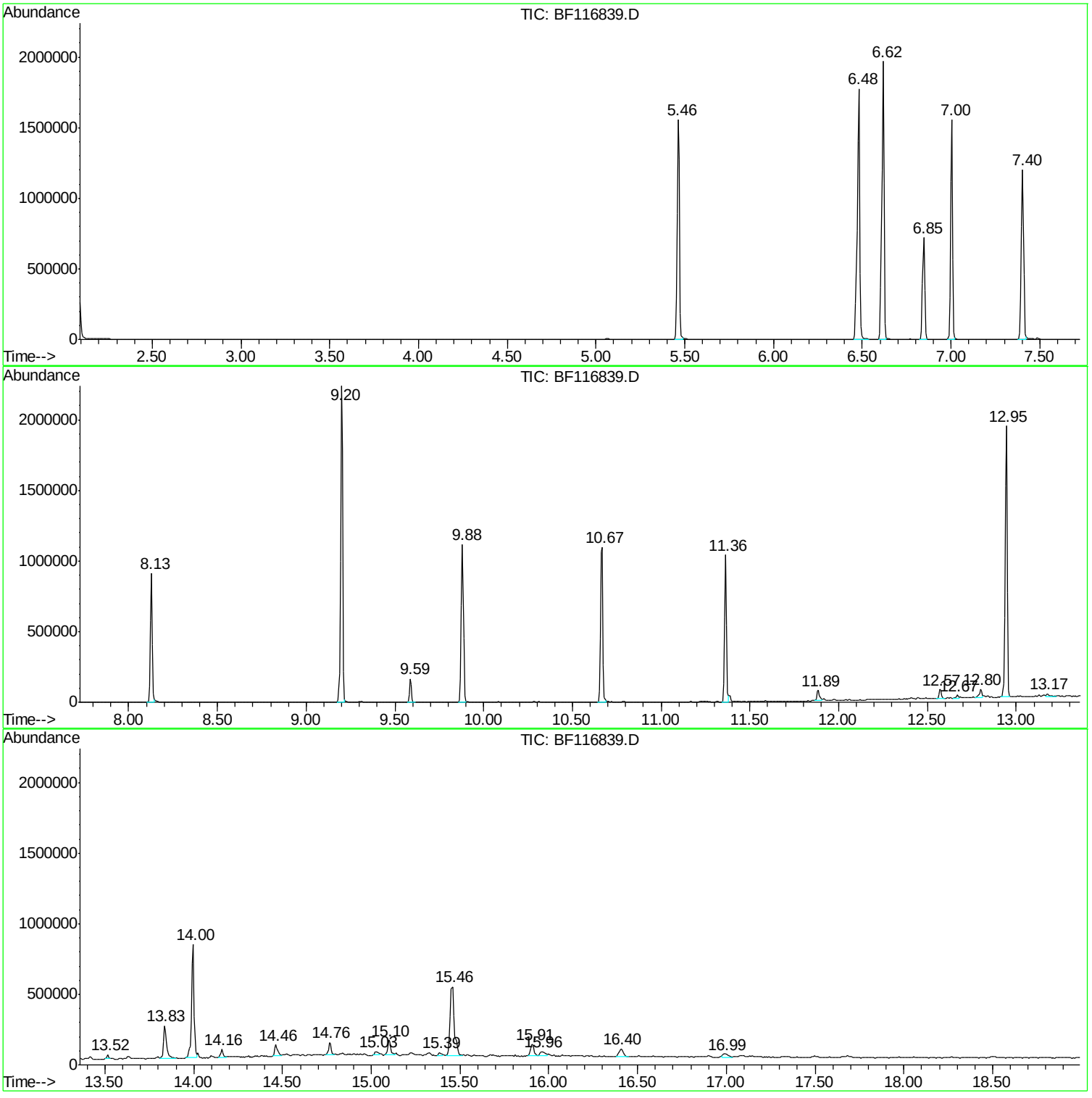
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

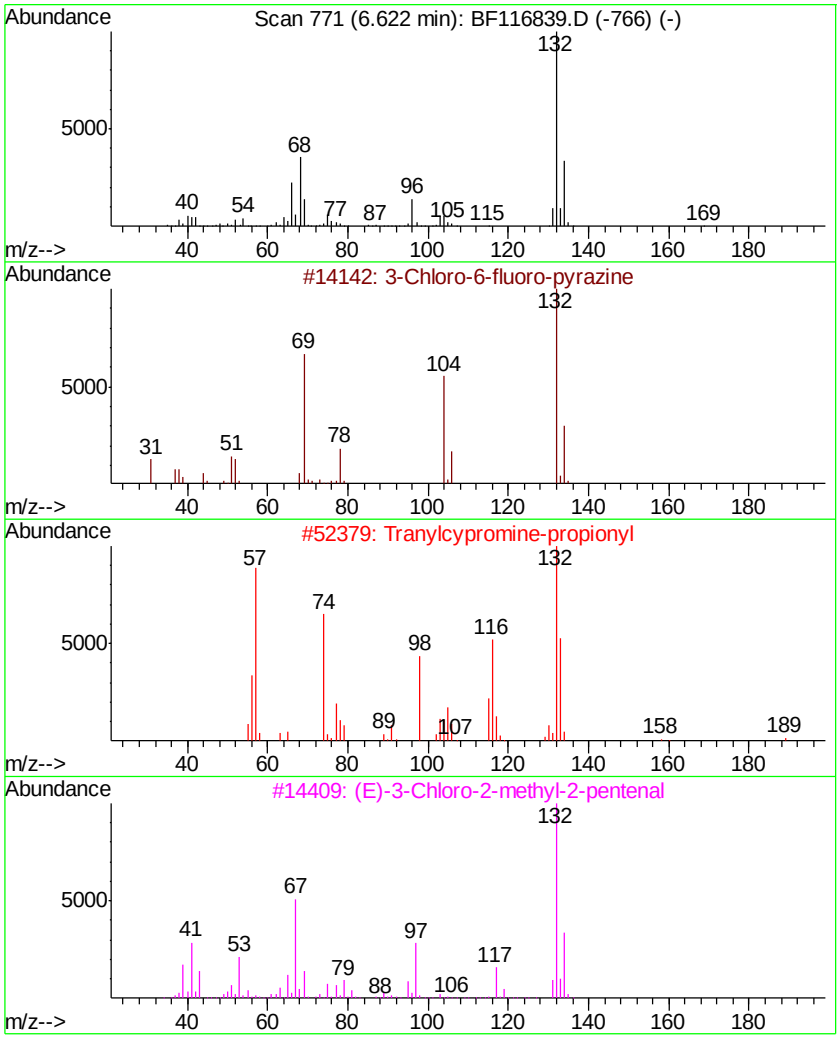
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

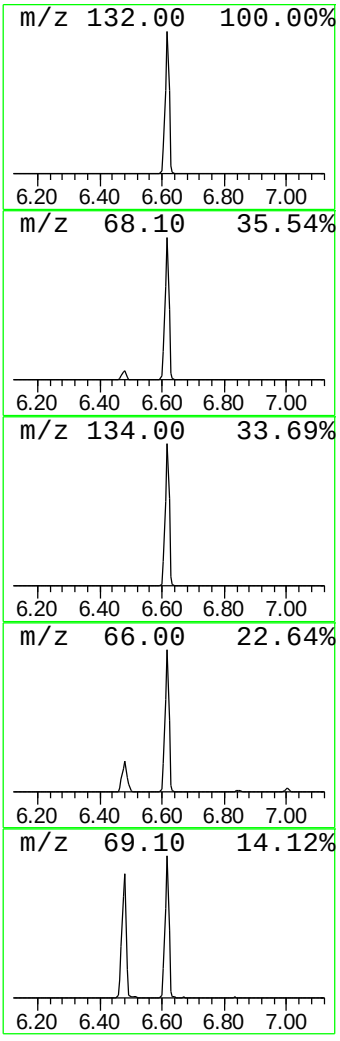
****

Peak Number 1 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	61.52 ng	1700050	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
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-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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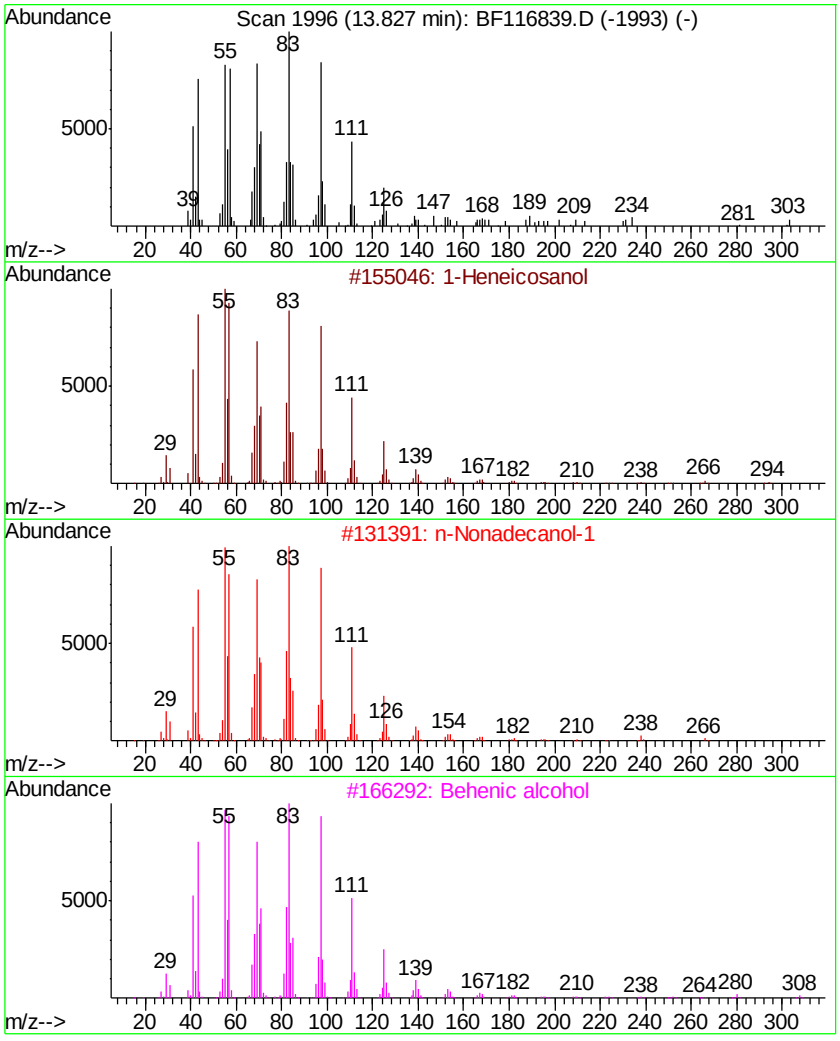
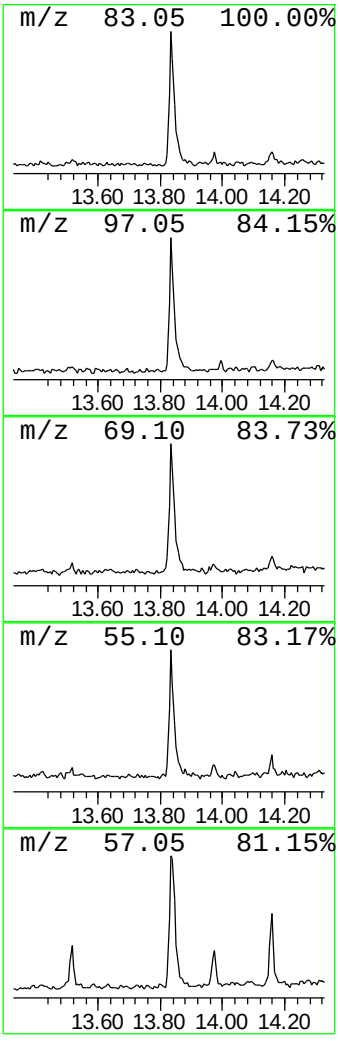
Peak Number 3 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	7.70 ng	312938	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5	3-Eicosene, (E)-	280	C20H40	074685-33-9	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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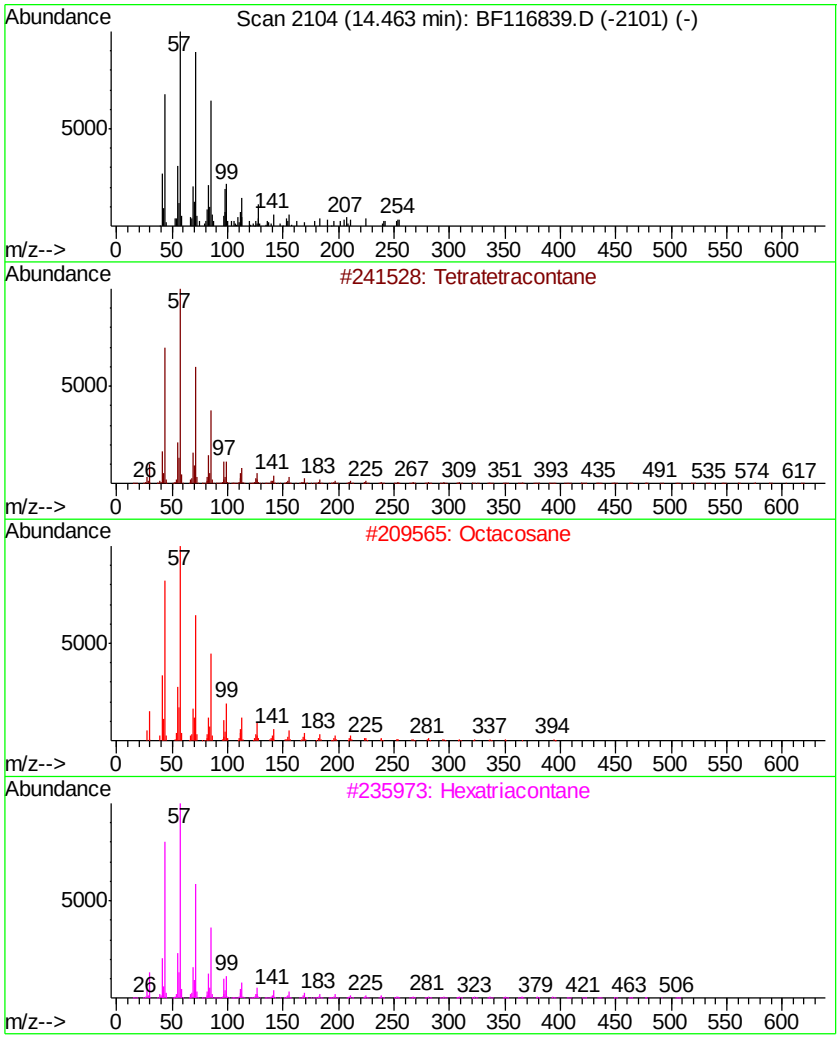
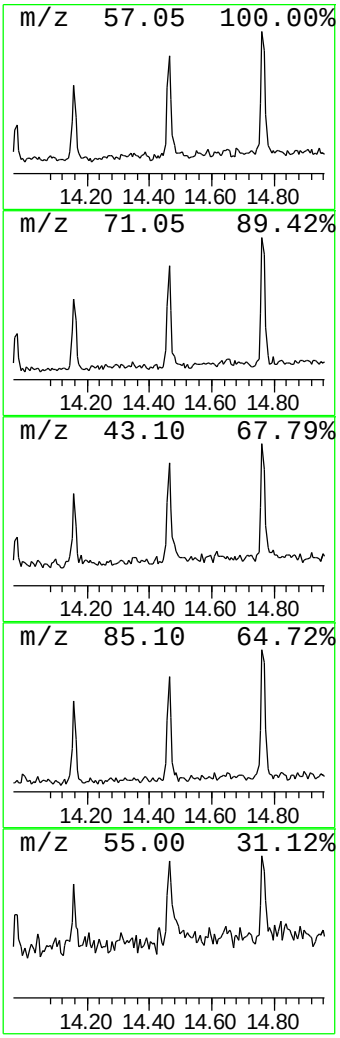
Peak Number 4 Tetratetracontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.46	2.01 ng	81646	Chrysene-d12	14.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Octacosane	394	C28H58	000630-02-4	87
3	Hexatriacontane	507	C36H74	000630-06-8	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	2-methyloctacosane	408	C29H60	1000376-72-8	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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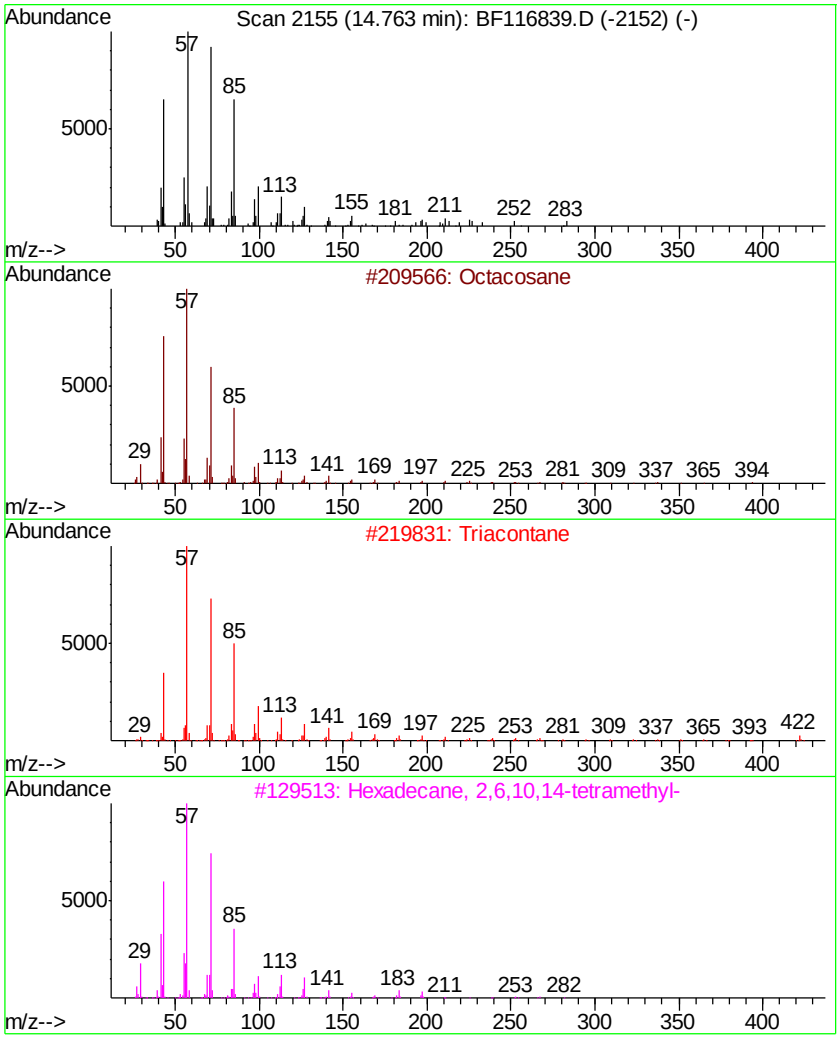
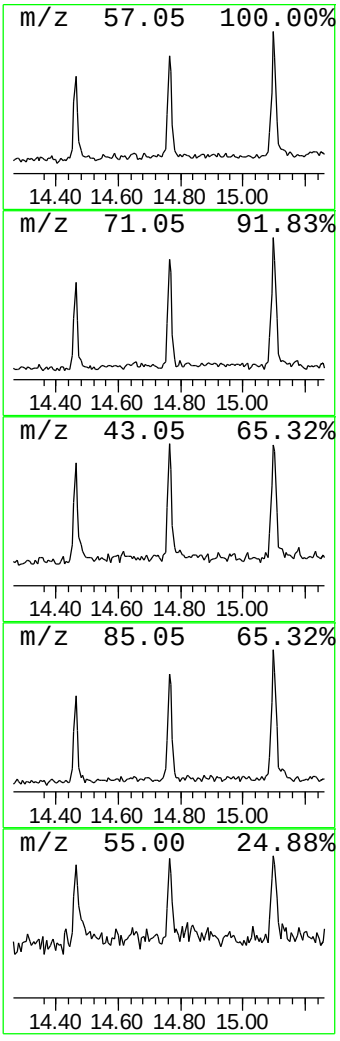
Peak Number 5 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.76	2.18 ng	81431	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Triacontane	422	C30H62	000638-68-6	91
3	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	90
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5	Hexacosane	366	C26H54	000630-01-3	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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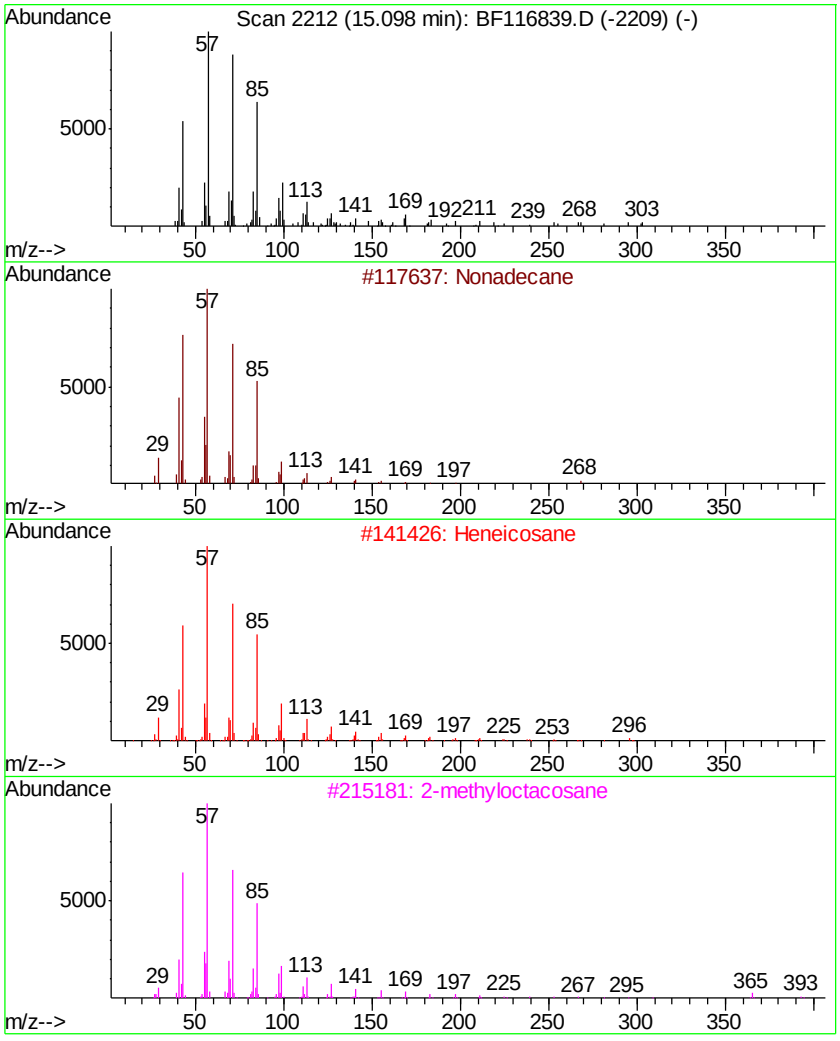
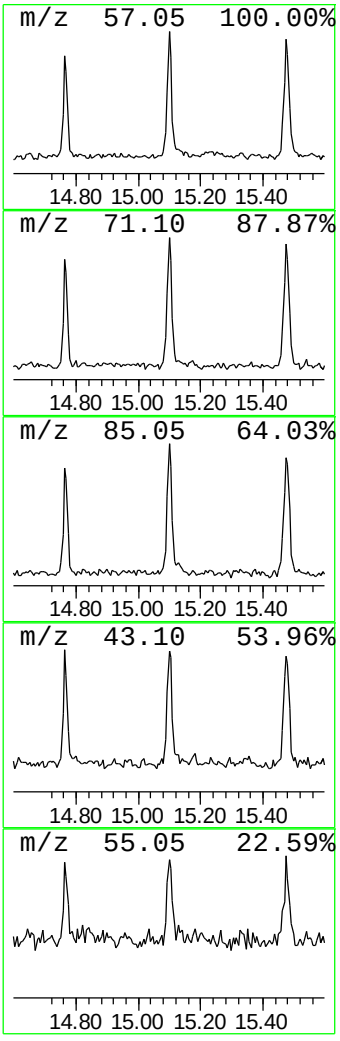
Peak Number 6 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	3.45 ng	128771	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Heptadecane	240	C17H36	000629-78-7	91
5	Hexacosane	366	C26H54	000630-01-3	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

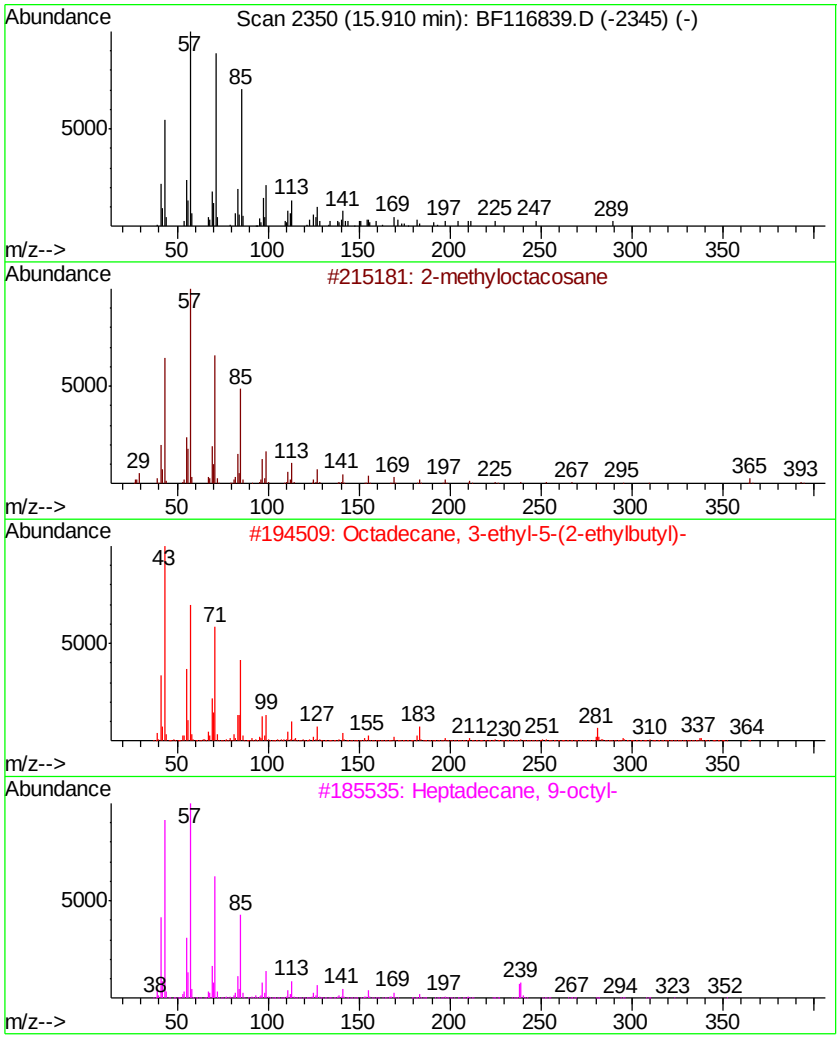
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

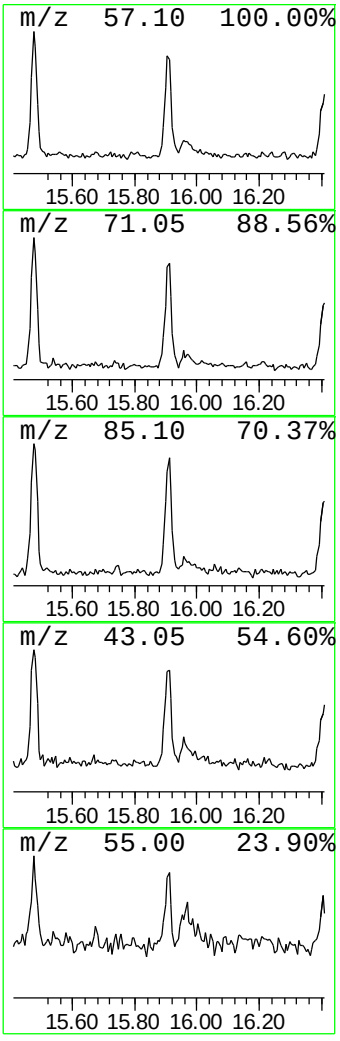
****

Peak Number 7 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.91	3.24 ng	121164	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	90
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	86





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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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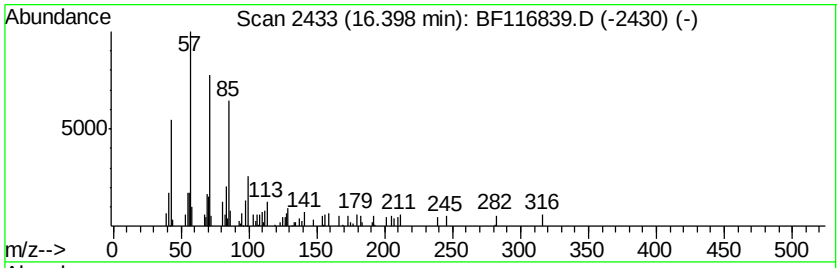
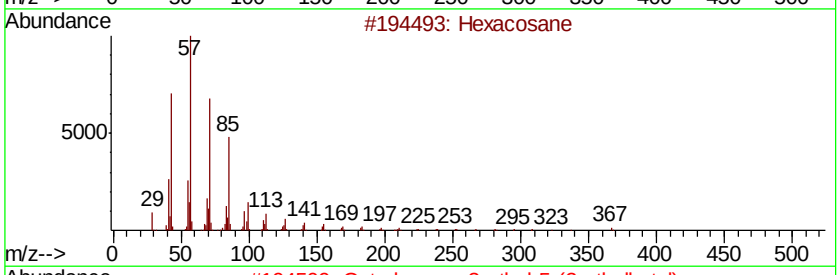
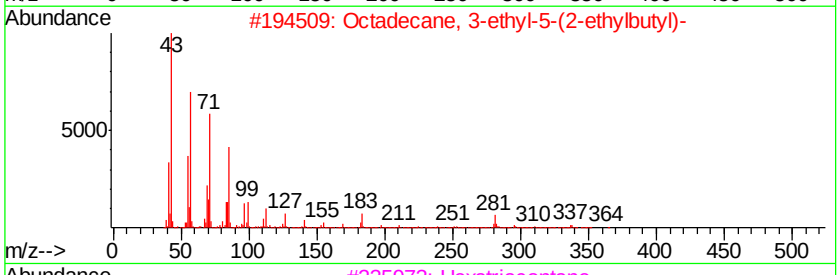
Peak Number 8 Hexacosane Concentration Rank 6

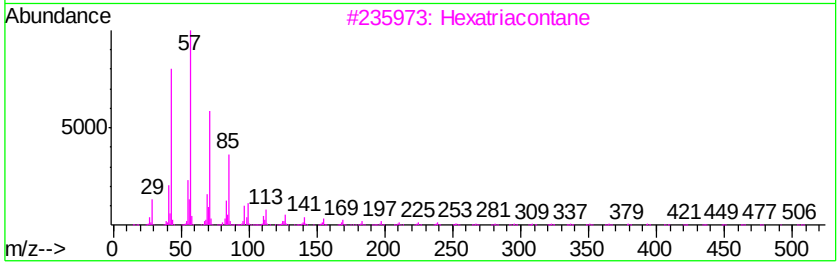
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.40	2.46 ng	91997	Perylene-d12	15.46

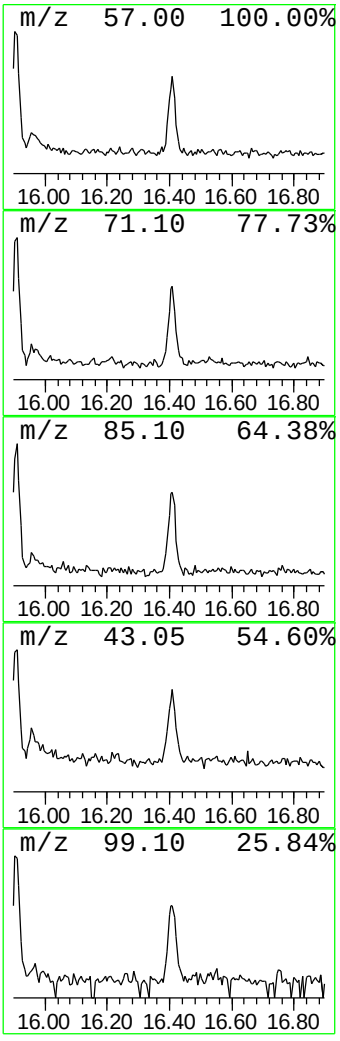
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	80
2	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	72
3	Hexatriacontane	507	C36H74	000630-06-8	72
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	64
5	Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	59











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF090519\
Data File : BF116839.D
Acq On : 5 Sep 2019 15:48
Operator : HP/JU
Sample : K4680-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T2-3-(2-4)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083019.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
unknown6.62	6.62	61.5	ng	1700050	1	6.85	552671	20.0
1-Heneicosanol	13.83	7.7	ng	312938	5	14.00	813083	20.0
Tetratetracontane	14.46	2.0	ng	81646	5	14.00	813083	20.0
Octacosane	14.76	2.2	ng	81431	6	15.46	747027	20.0
Nonadecane	15.10	3.5	ng	128771	6	15.46	747027	20.0
2-methyloctacosane	15.91	3.2	ng	121164	6	15.46	747027	20.0
Hexacosane	16.40	2.5	ng	91997	6	15.46	747027	20.0