LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117036.D
Acq On : 13 Sep 2019 21:32
Operator : HP/JU
Sample : K4848-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-C

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	585	rBV	772163	837002	31.75%	4.951%
2	6.451	738	742	756	rBV	584535	596856	22.64%	3.530%
3	6.592	762	766	769	rBV	2018574	1727259	65.52%	10.216%
4	6.822	801	805	814	rBV	488448	409761	15.54%	2.424%
5	6.981	827	832	835	rBV	1850479	1613149	61.20%	9.541%
6	7.381	896	900	917	rBV	1227661	1344262	51.00%	7.951%
7	8.104	1019	1023	1039	rBV	473467	525358	19.93%	3.107%
8	9.175	1201	1205	1208	rBV	2869980	2508309	95.15%	14.836%
9	9.563	1268	1271	1279	rBV	137739	143072	5.43%	0.846%
10	9.851	1316	1320	1333	rBV	678551	625218	23.72%	3.698%
11	10.492	1426	1429	1437	rBV	25630	32013	1.21%	0.189%
12	10.639	1449	1454	1460	rBV	1632436	1565458	59.39%	9.259%
13	10.692	1460	1463	1478	rVB	80358	158477	6.01%	0.937%
14	11.333	1568	1572	1585	rBV	634126	622465	23.61%	3.682%
15	11.857	1658	1661	1671	rBV	118662	128625	4.88%	0.761%
16	12.639	1791	1794	1804	rBV	61224	76271	2.89%	0.451%
17	12.916	1836	1841	1844	rBV	2806179	2636046	100.00%	15.591%
18	13.816	1990	1994	2006	rBV6	39282	99403	3.77%	0.588%
19	13.963	2015	2019	2031	rVB	467772	544889	20.67%	3.223%
20	14.427	2094	2098	2102	rBV2	36012	38825	1.47%	0.230%
21	14.727	2146	2149	2153	rBV	48226	43301	1.64%	0.256%
22	15.057	2200	2205	2210	rBV	51615	61699	2.34%	0.365%
23	15.410	2260	2265	2275	rBV	321431	475811	18.05%	2.814%
24	15.845	2334	2339	2348	rBV	37576	55279	2.10%	0.327%
25	16.333	2414	2422	2428	rBV2	21665	38259	1.45%	0.226%

Sum of corrected areas: 16907067

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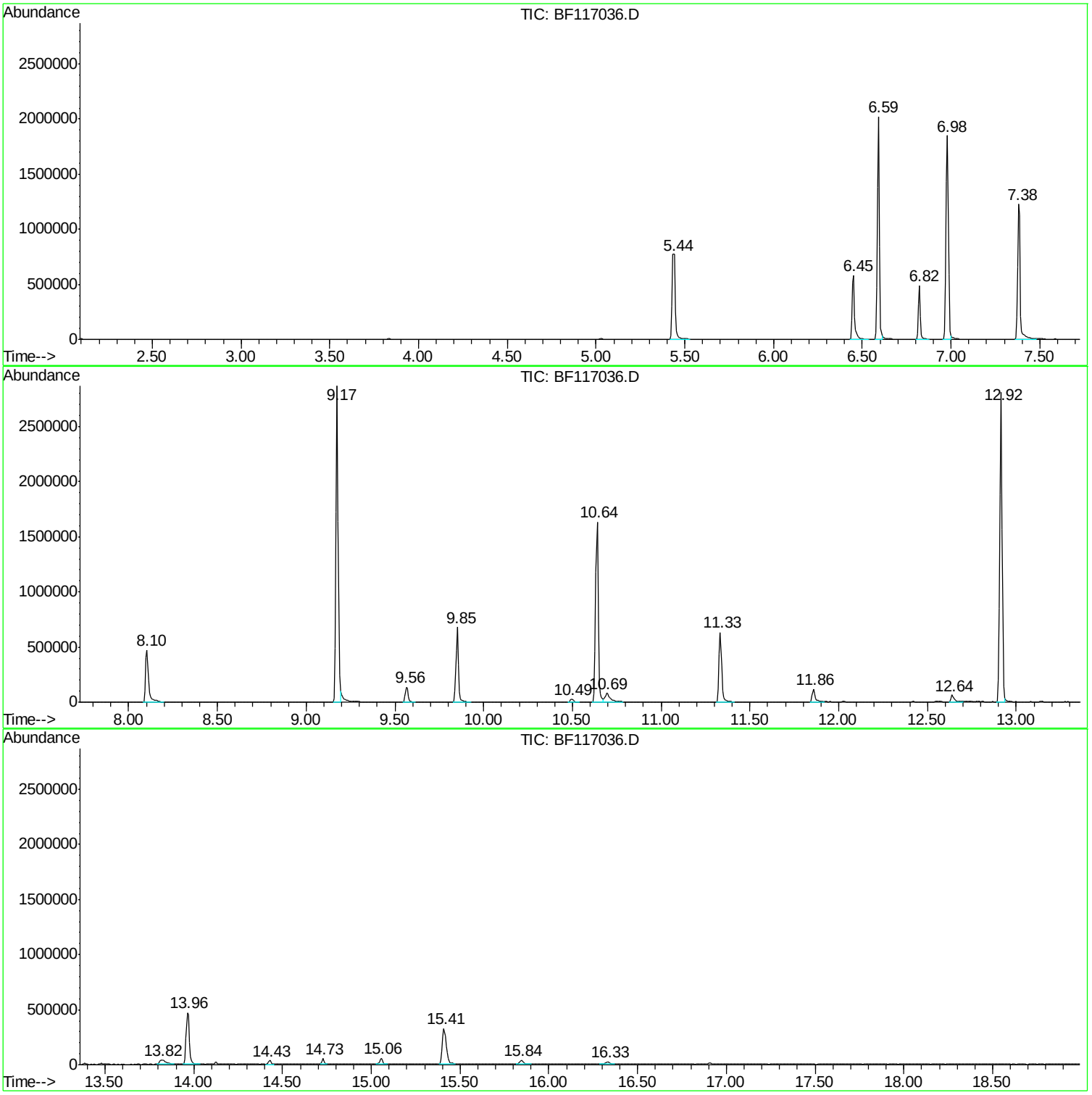
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CBH-139-C

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117036.D
Acq On : 13 Sep 2019 21:32
Operator : HP/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : CBH-139-C

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

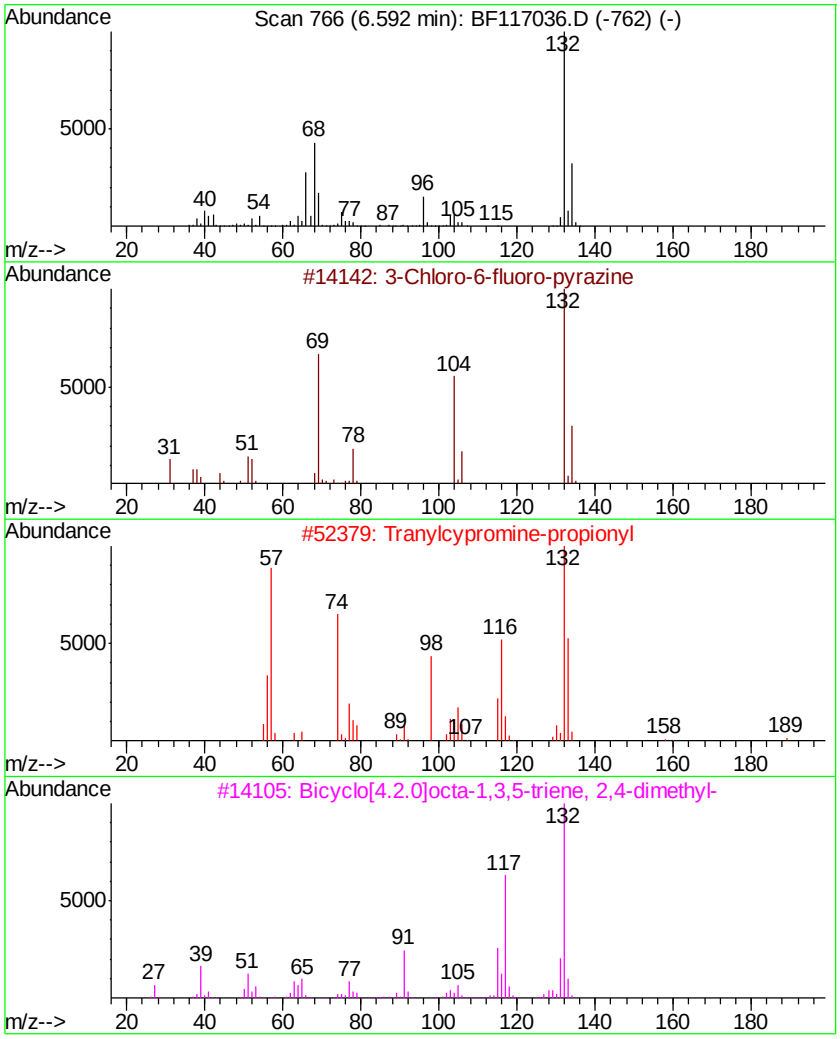
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

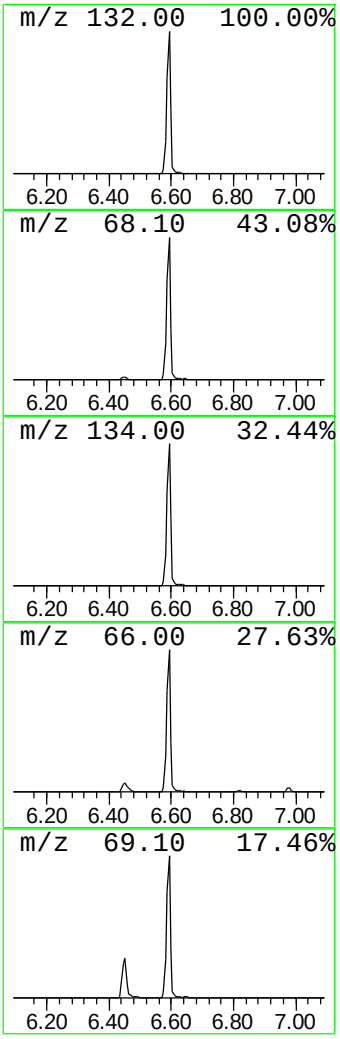
****

Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	84.31 ng	1727260	1,4-Dichlorobenzene-d4	6.82

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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9





Library Search Compound Report

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Data File : BF117036.D
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Operator : HP/JU
Sample : K4848-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-C

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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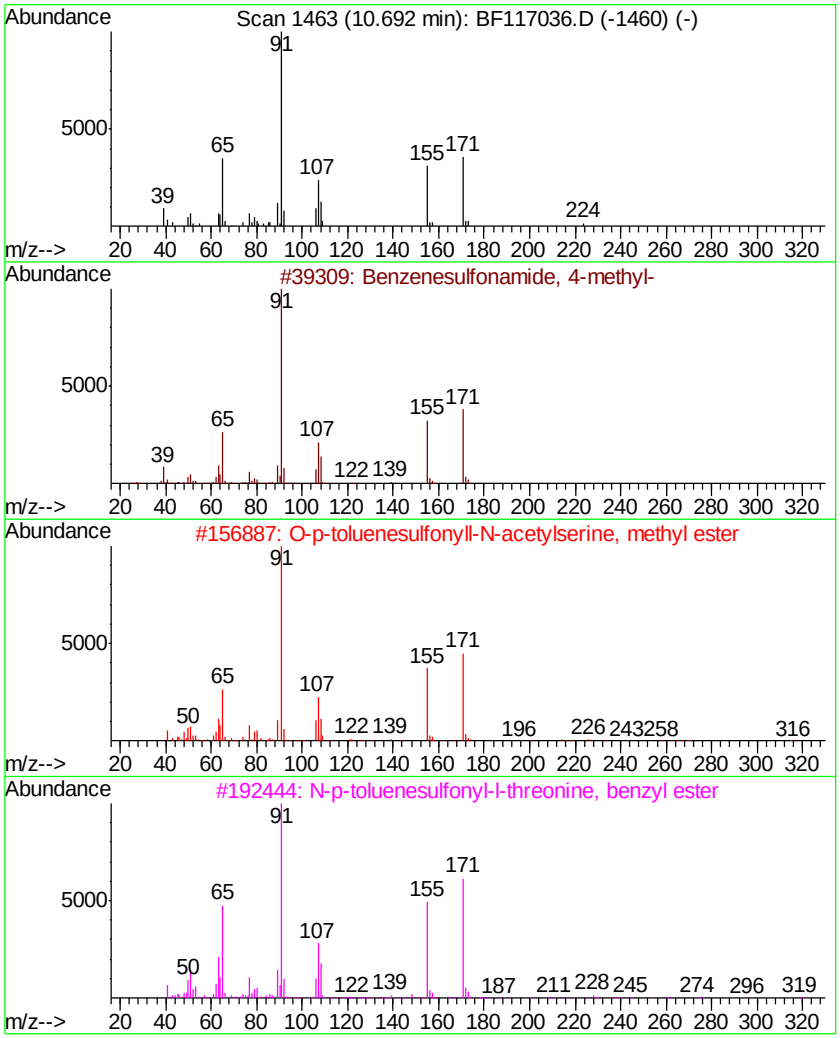
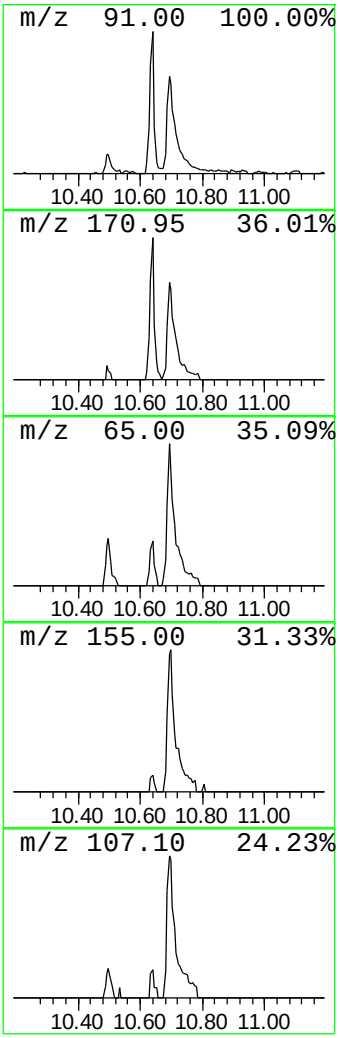
Peak Number 3 Benzenesulfonamide, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	5.09 ng	158477	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	94
2	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	90
3	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	64
4	Tolbutamide	270	C12H18N2O3S	000064-77-7	53
5	Thiophene-3-ol, 2,3-dihydro-, 4-...	288	C11H12O5S2	039582-96-2	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
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Sample : K4848-03
Misc :
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Instrument : BNA_F
ClientSampleId : CBH-139-C

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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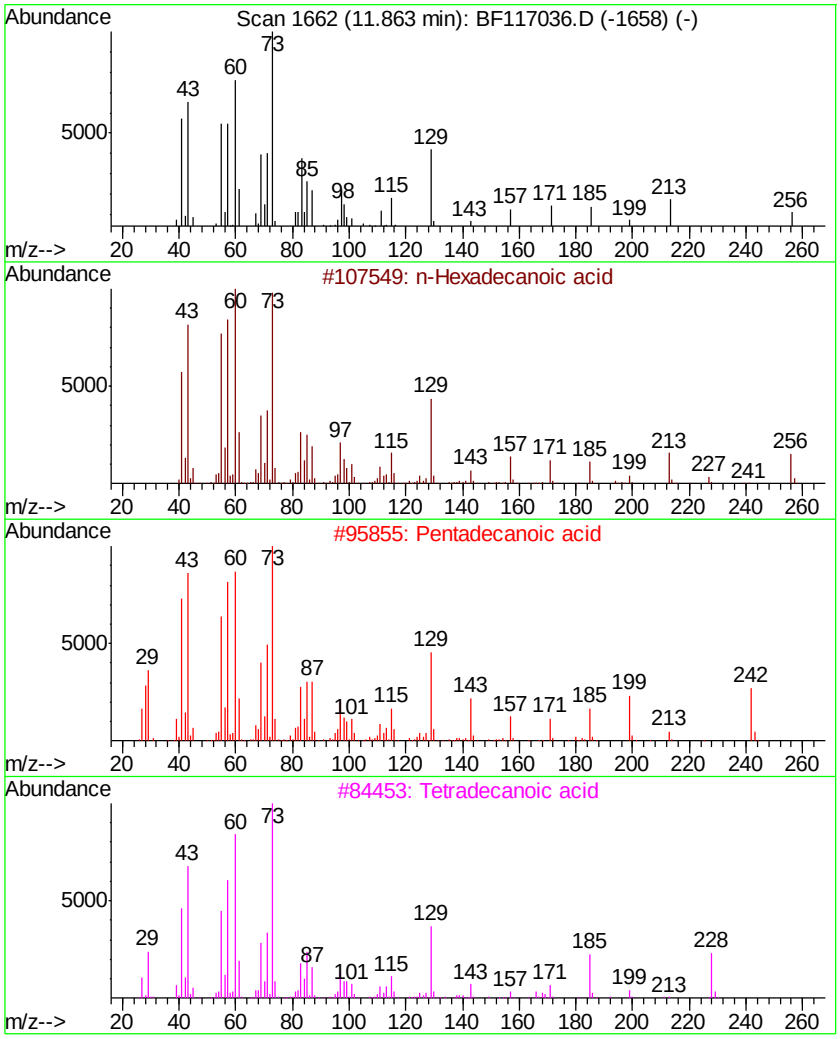
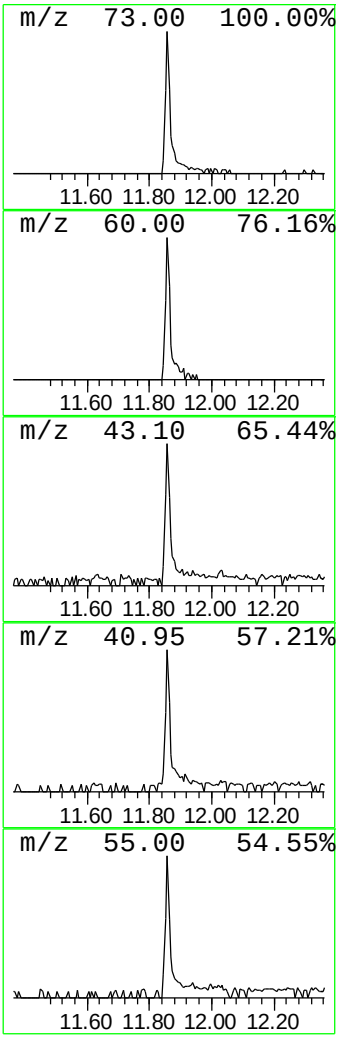
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	4.13 ng	128625	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	30
5	Sulfurous acid, 2-propyl tetrade...	320	C17H36O3S	1000309-12-5	25





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117036.D
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Operator : HP/JU
Sample : K4848-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-C

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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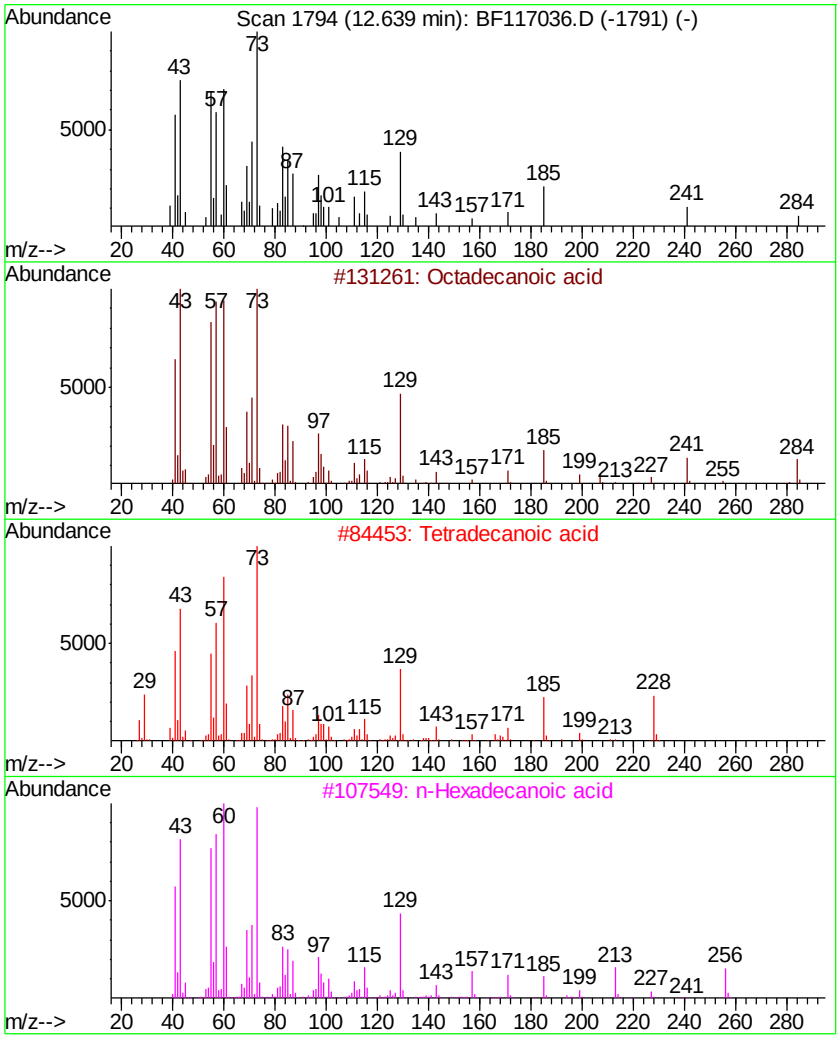
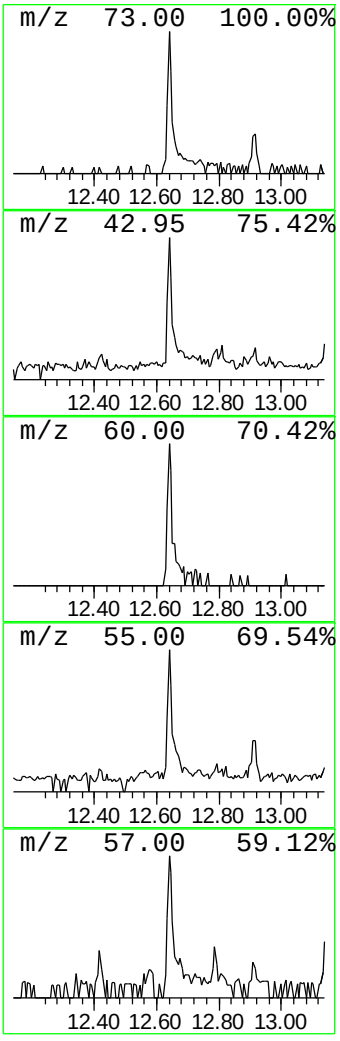
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.64	2.45 ng	76271	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52
4	Cyclohexane, (1-hexyltetradecyl)-	364	C26H52	004443-60-1	38
5	n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
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Misc :
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Instrument : BNA_F
ClientSampleId : CBH-139-C

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

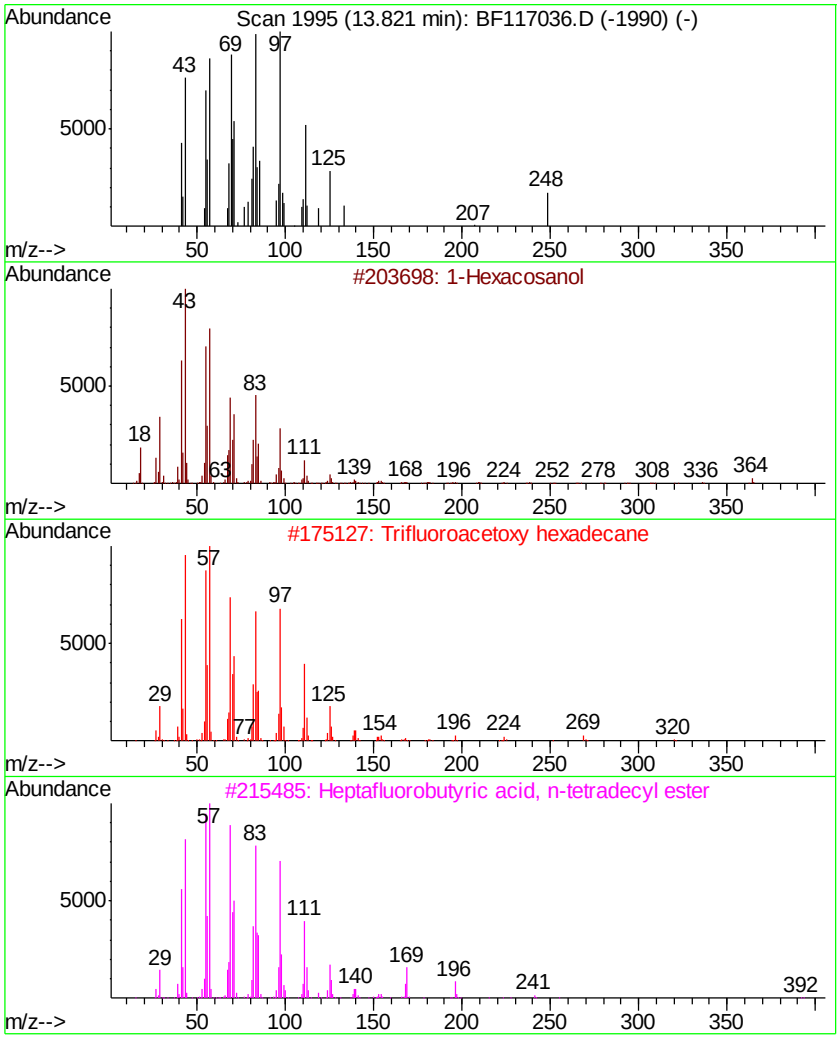
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

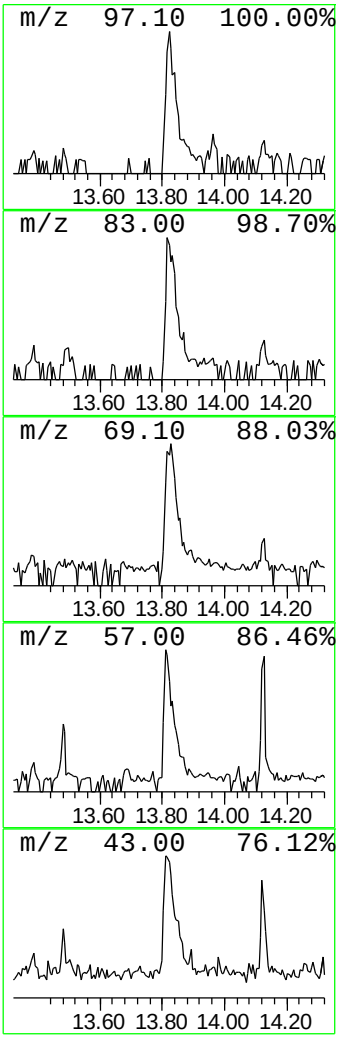
****

Peak Number 6 1-Hexacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.65 ng	99403	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	91
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
4	1-Heptacosanol	396	C27H56O	002004-39-9	87
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87





Library Search Compound Report

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Data File : BF117036.D
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Operator : HP/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

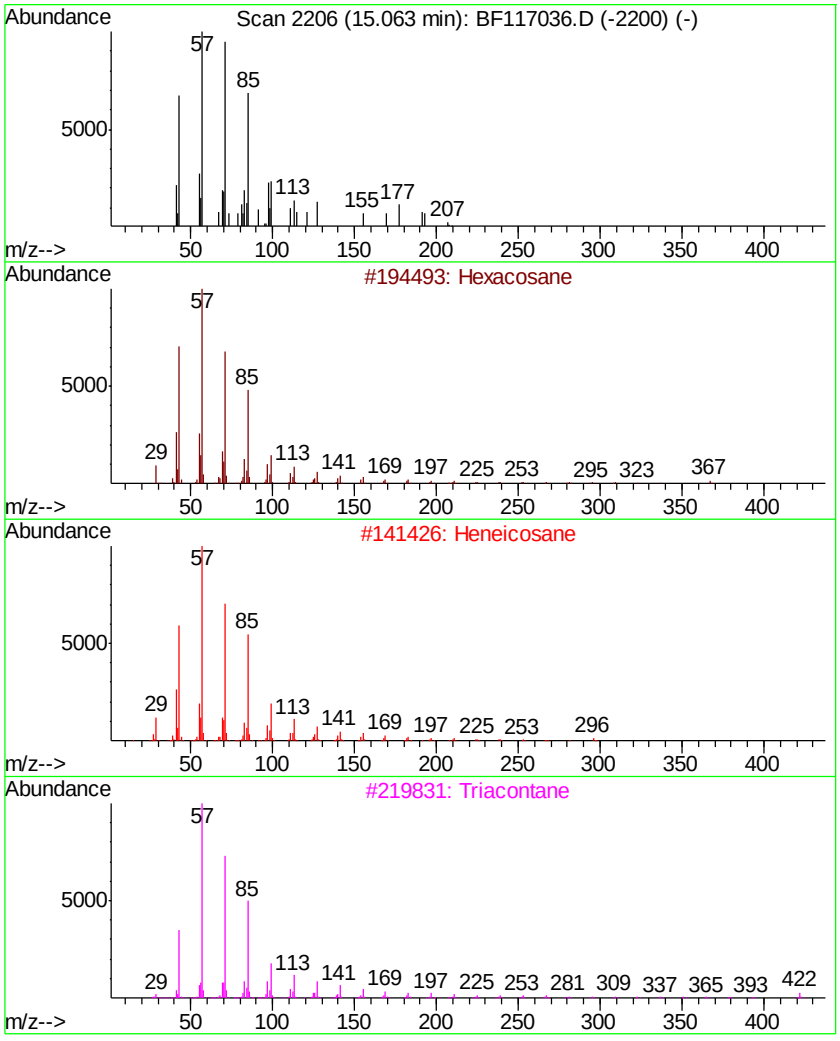
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

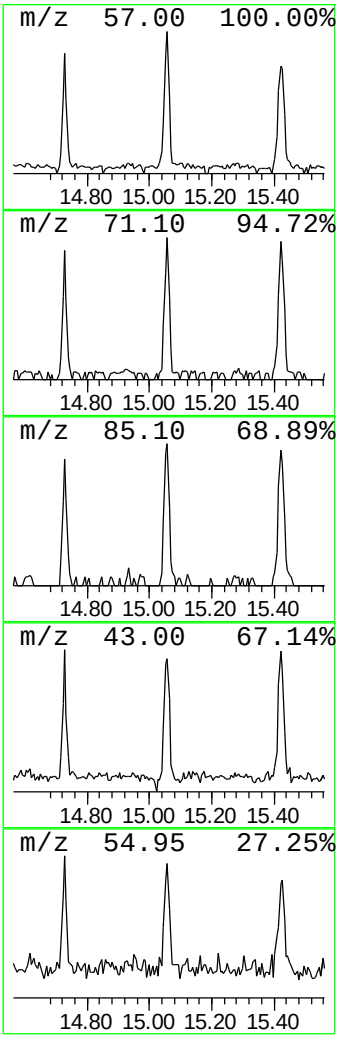
****

Peak Number 7 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	2.59 ng	61699	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Triacontane	422	C30H62	000638-68-6	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Octacosane	394	C28H58	000630-02-4	87





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Operator : HP/JU
Sample : K4848-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-C

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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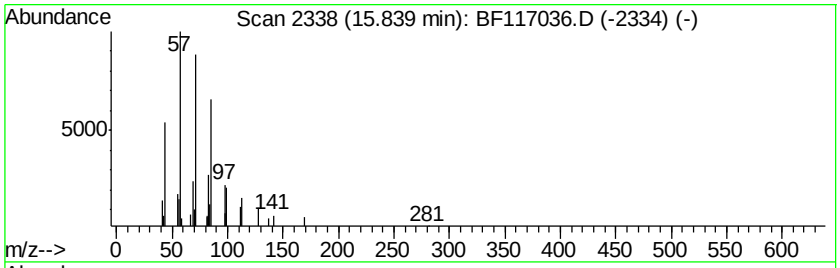
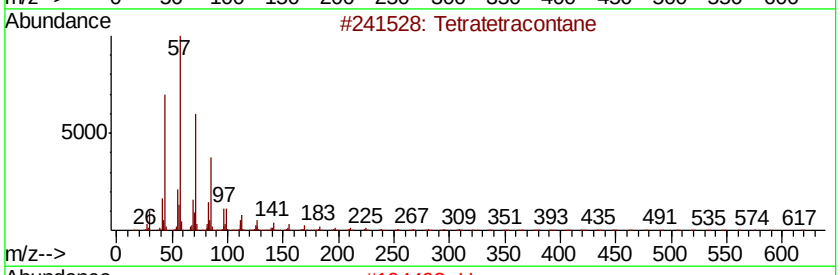
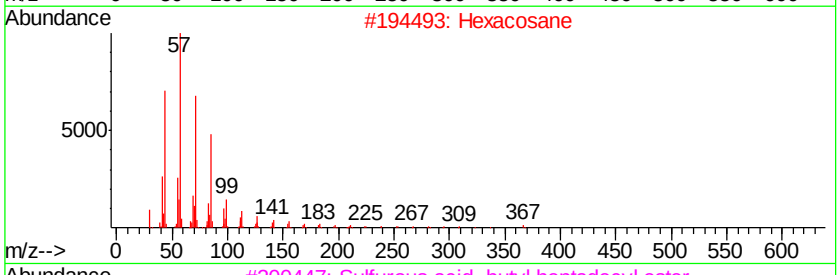
Peak Number 8 Tetratetracontane Concentration Rank 8

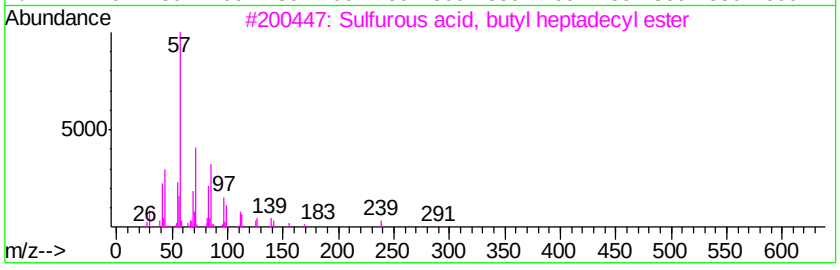
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.32 ng	55279	Perylene-d12	15.41

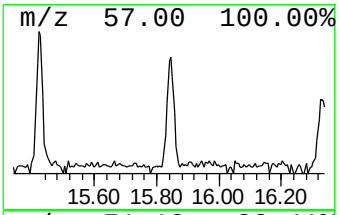
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	90
2	Hexacosane	366	C26H54	000630-01-3	87
3	Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	86
4	Heneicosane	296	C21H44	000629-94-7	80
5	Octadecane	254	C18H38	000593-45-3	72

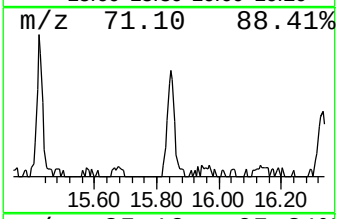


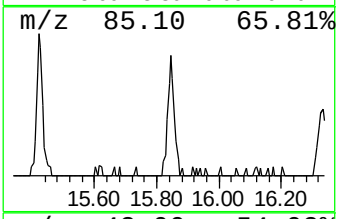


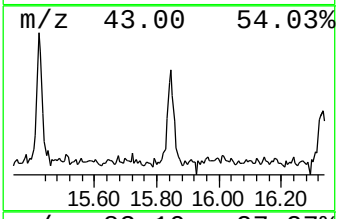


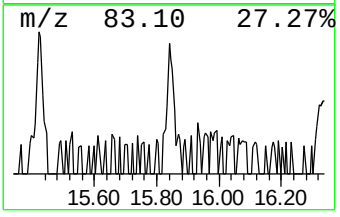












Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091319\
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Misc :
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Instrument : BNA_F
ClientSampleId : CBH-139-C

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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
unknown6.59	6.59	84.3	ng	1727260	1	6.82	409761	20.0
Benzenesulfonamid...	10.69	5.1	ng	158477	4	11.33	622465	20.0
n-Hexadecanoic acid	11.86	4.1	ng	128625	4	11.33	622465	20.0
Octadecanoic acid	12.64	2.5	ng	76271	4	11.33	622465	20.0
1-Hexacosanol	13.82	3.6	ng	99403	5	13.96	544889	20.0
Hexacosane	15.06	2.6	ng	61699	6	15.41	475811	20.0
Tetratetracontane	15.84	2.3	ng	55279	6	15.41	475811	20.0