LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

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-BF111319.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	2.169	8	14	30	rVB	665835	943260	21.45%	2.424%
2	5.116	507	515	523	rBV	523660	650348	14.79%	1.671%
3	5.516	578	583	586	rBV	3283954	3230270	73.45%	8.300%
4	6.528	749	755	758	rBV	3331547	3338357	75.91%	8.578%
5	6.675	775	780	783	rBV	3531781	3576601	81.33%	9.190%
6	6.904	815	819	822	rBV	970475	810069	18.42%	2.082%
7	7.063	841	846	849	rBV	3076555	2789049	63.42%	7.167%
8	7.463	909	914	917	rBV	2204309	2243139	51.01%	5.764%
9	8.192	1034	1038	1041	rBV	963124	925041	21.03%	2.377%
10	9.269	1216	1221	1224	rBV	4678180	4211735	95.77%	10.822%
11	9.663	1284	1288	1298	rVB	686149	606477	13.79%	1.558%
12	9.851	1316	1320	1333	rBV4	19065	45746	1.04%	0.118%
13	9.951	1333	1337	1341	rBV	1560351	1301622	29.60%	3.345%
14	10.745	1467	1472	1475	rBV	3347277	3020377	68.68%	7.761%
15	11.445	1587	1591	1594	rBV	1600358	1397213	31.77%	3.590%
16	11.510	1598	1602	1605	rVB2	55888	62168	1.41%	0.160%
17	11.969	1674	1680	1694	rBV	620629	627697	14.27%	1.613%
18	12.663	1795	1798	1810	rBV	78462	102164	2.32%	0.263%
19	12.751	1810	1813	1822	rBV	205838	221244	5.03%	0.568%
20	12.892	1835	1837	1841	rVB2	43669	44624	1.01%	0.115%
21	13.039	1857	1862	1865	rBV	4681010	4397730	100.00%	11.300%
22	13.604	1952	1958	1961	rBV2	58140	59780	1.36%	0.154%
23	13.927	2009	2013	2025	rBV2	373196	509771	11.59%	1.310%
24	14.092	2037	2041	2044	rBV	1567356	1410590	32.08%	3.625%
25	14.251	2063	2068	2071	rBV	142626	132561	3.01%	0.341%
26	14.557	2116	2120	2127	rBV	188485	192087	4.37%	0.494%
27	14.874	2168	2174	2178	rBV	153231	165154	3.76%	0.424%
28	14.951	2183	2187	2191	rVB	131508	145671	3.31%	0.374%
29	15.227	2229	2234	2238	rBV	163209	187066	4.25%	0.481%
30	15.598	2291	2297	2300	rBV	814657	1044554	23.75%	2.684%
31	16.080	2374	2379	2384	rBV	121649	173240	3.94%	0.445%
32	16.139	2384	2389	2397	rBV6	23564	53186	1.21%	0.137%
33	16.604	2462	2468	2476	rBV	78376	148910	3.39%	0.383%
34	17.227	2568	2574	2581	rVB2	42989	92355	2.10%	0.237%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
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Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

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-BF111319.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.956	2695	2698	2707	rVB5	25694	57362	1.30%	0.147%

Sum of corrected areas: 38917218

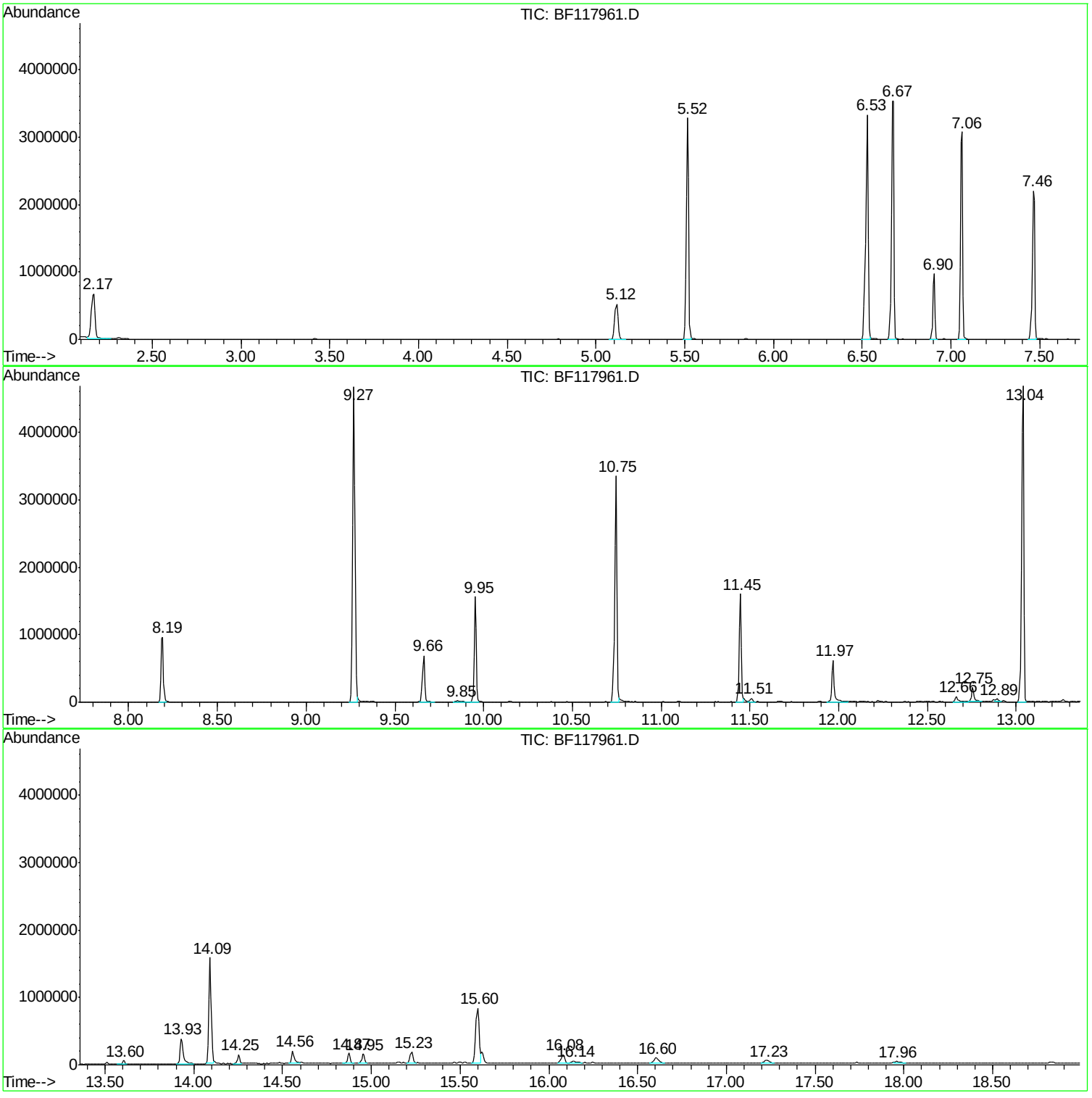
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

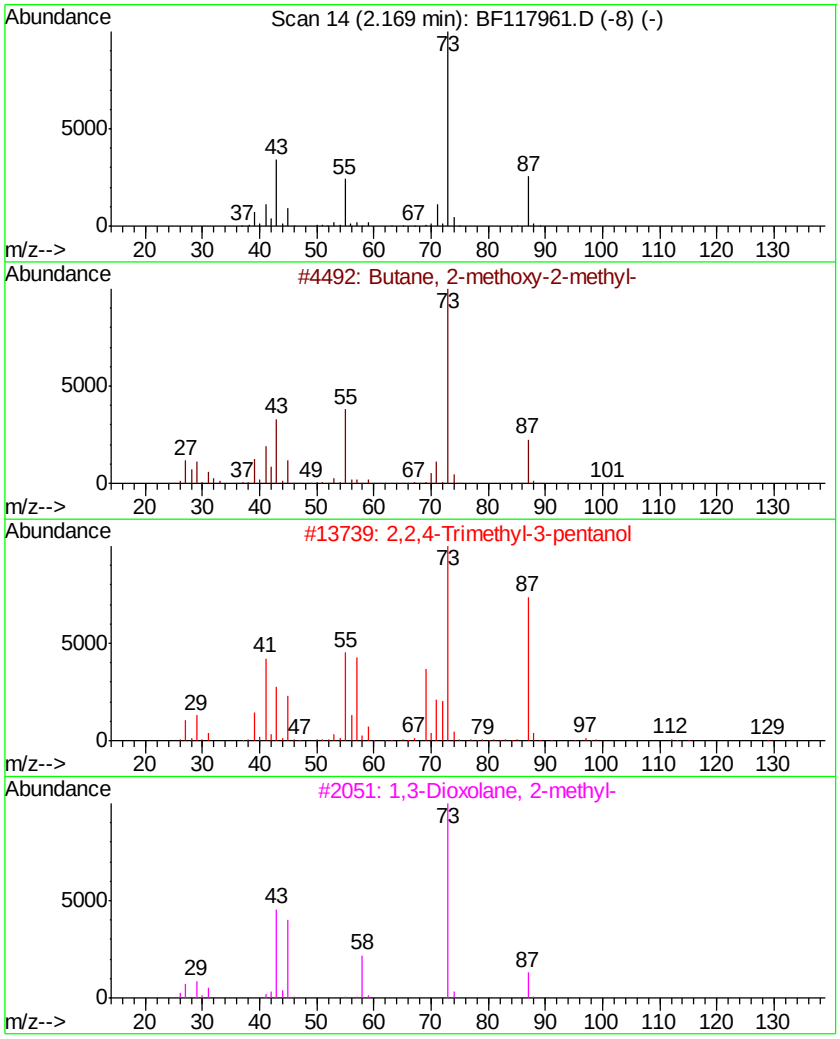
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

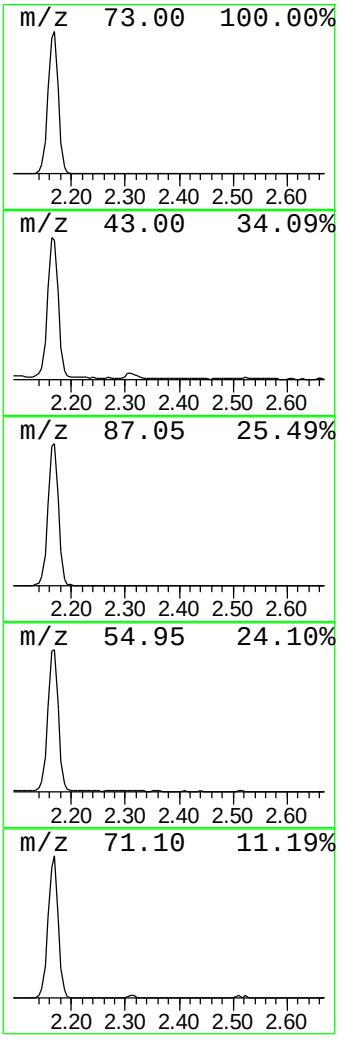
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	23.29 ng	943260	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

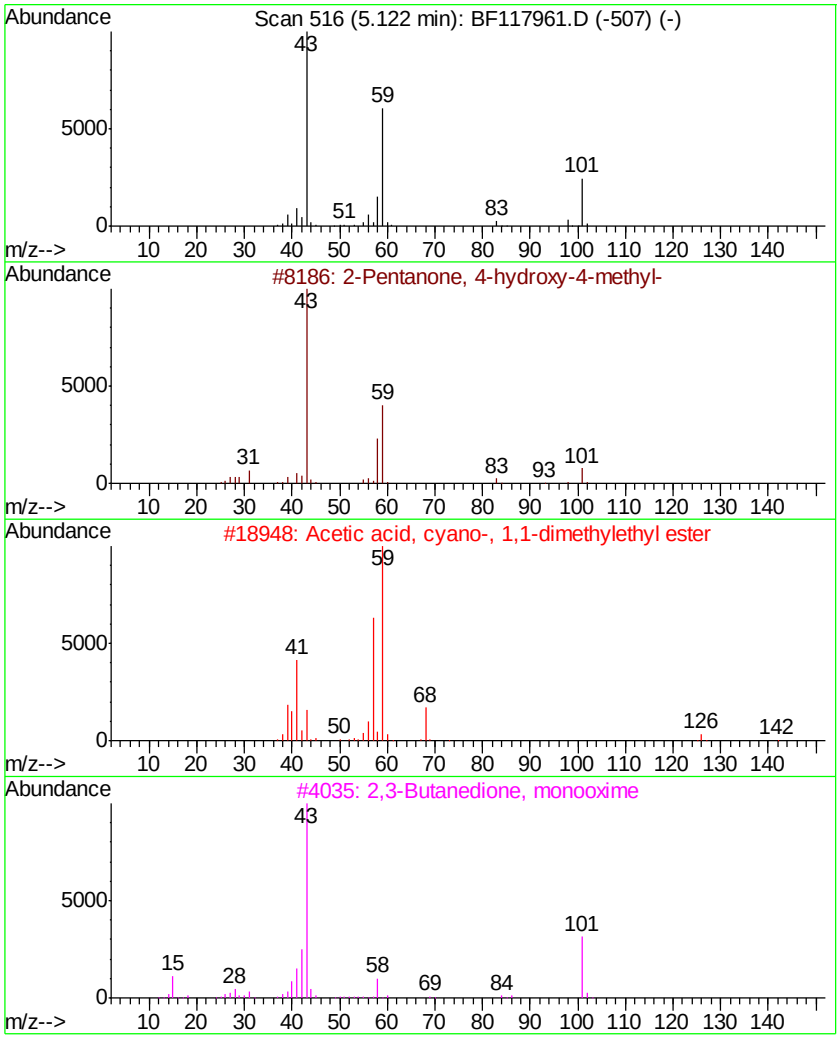
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

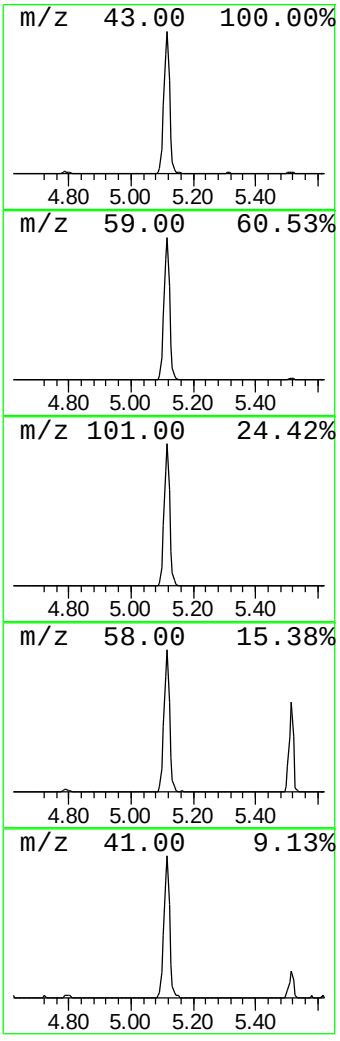
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	16.06 ng	650348	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

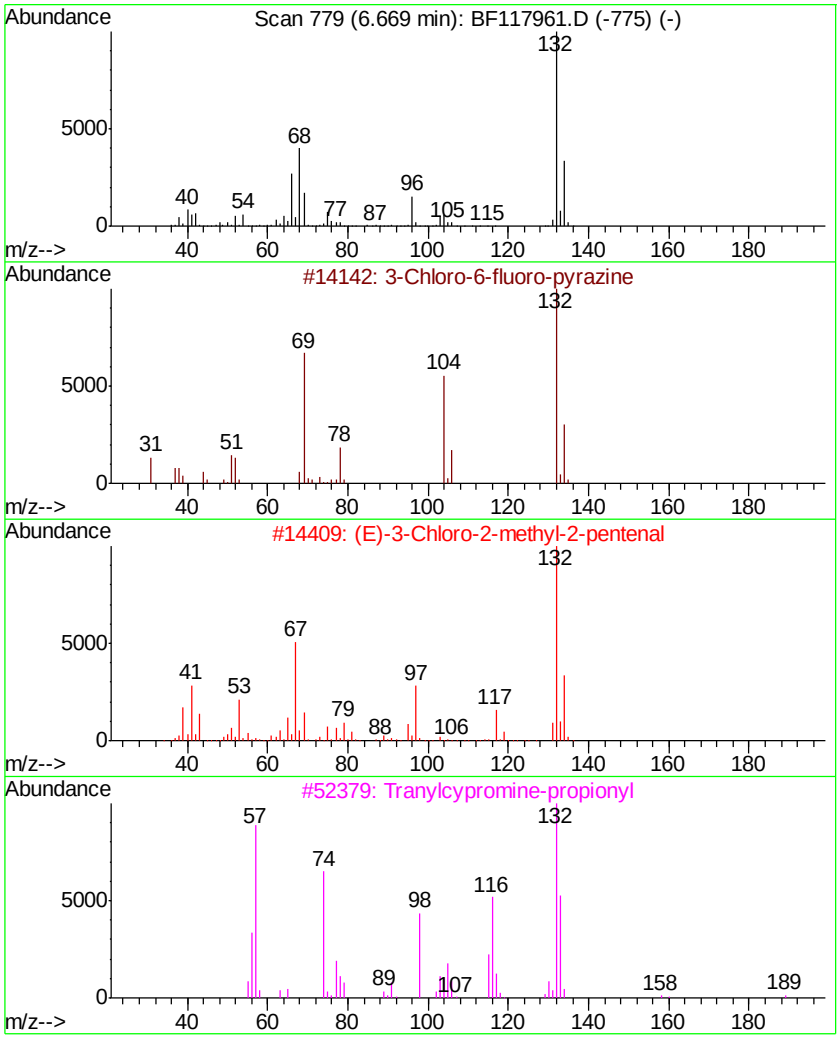
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

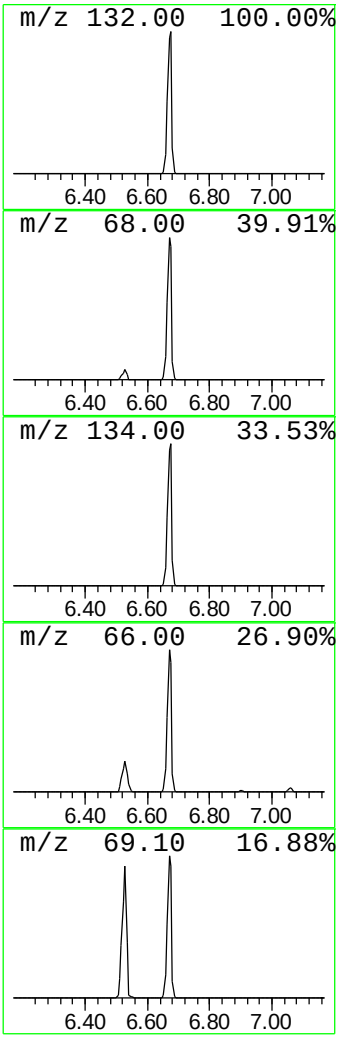
****

Peak Number 3 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	88.30 ng	3576600	1,4-Dichlorobenzene-d4	6.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	16
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

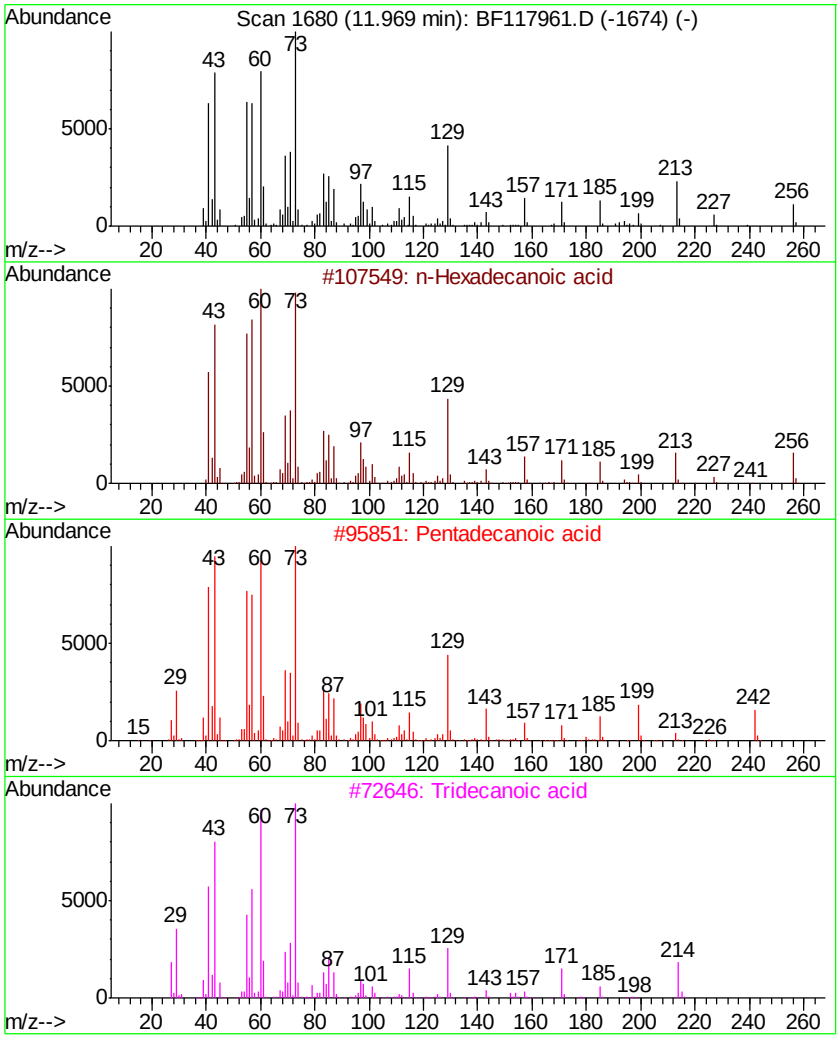
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

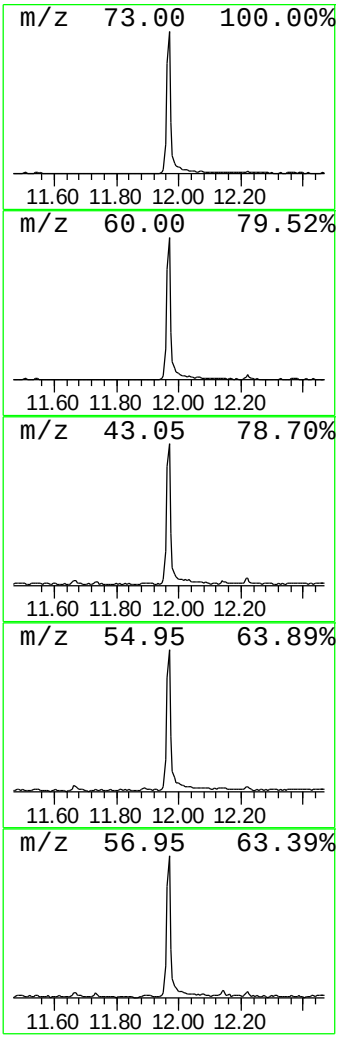
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.97	8.98 ng	627697	Phenanthrene-d10	11.45

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	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





Library Search Compound Report

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Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

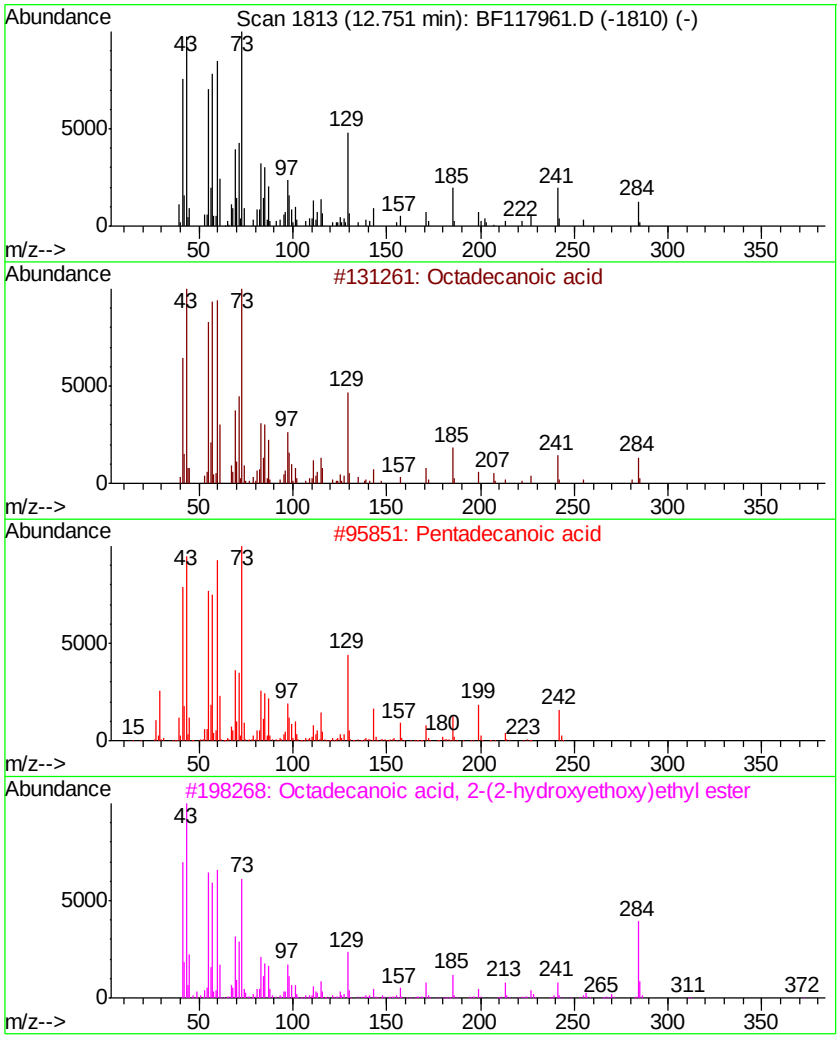
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

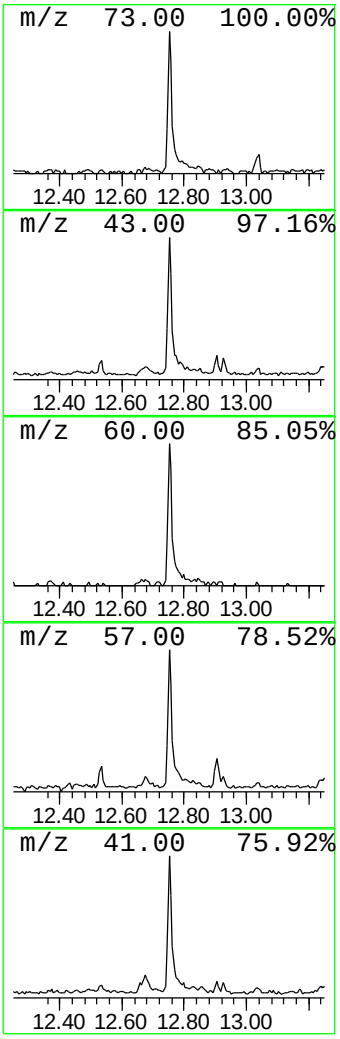
****

Peak Number 6 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	3.17 ng	221244	Phenanthrene-d10	11.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83





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Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

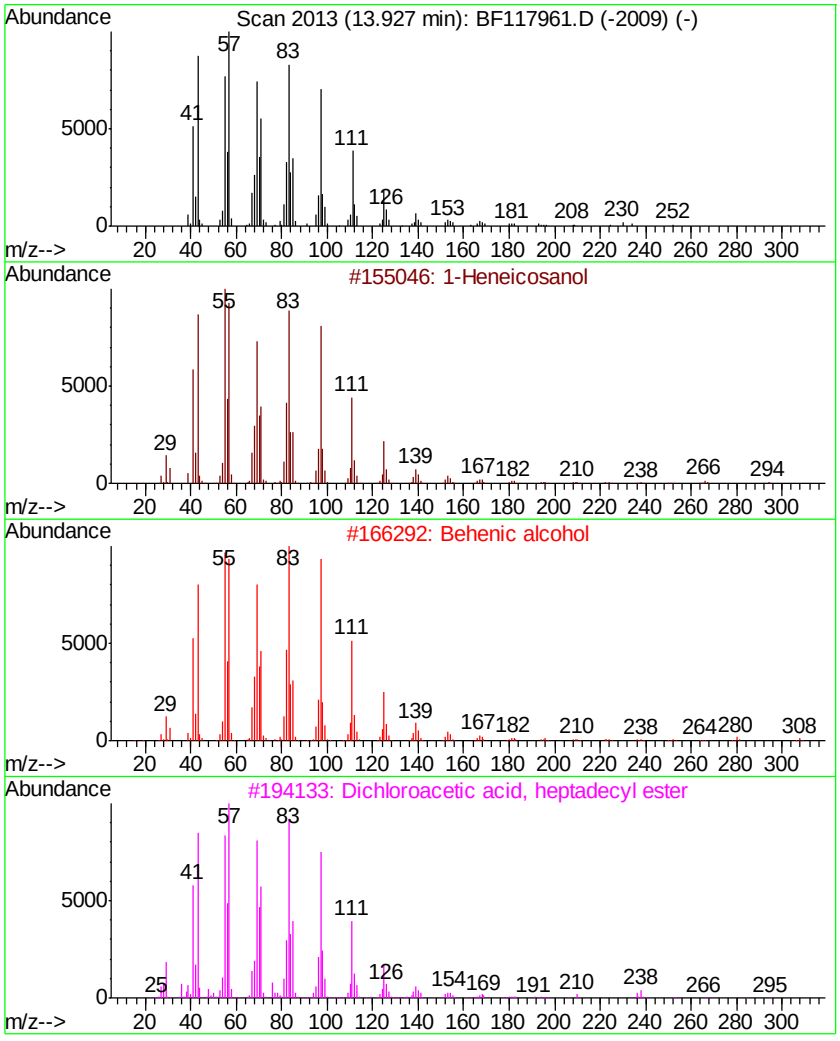
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

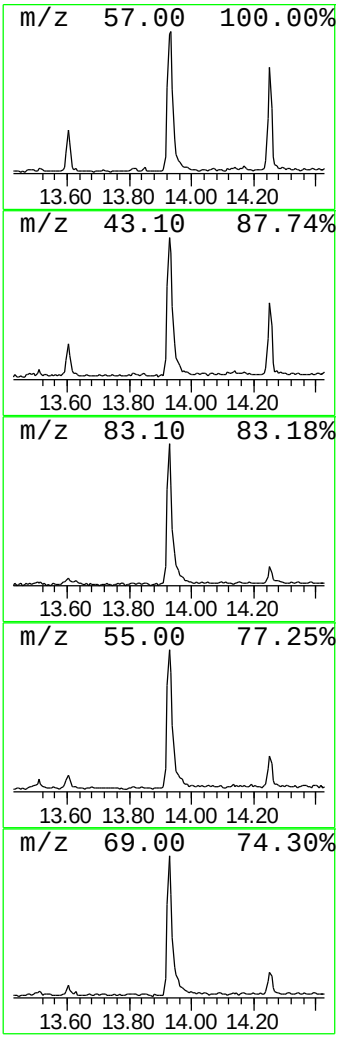
****

Peak Number 7 1-Heneicosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	7.23 ng	509771	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	94





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Misc :
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Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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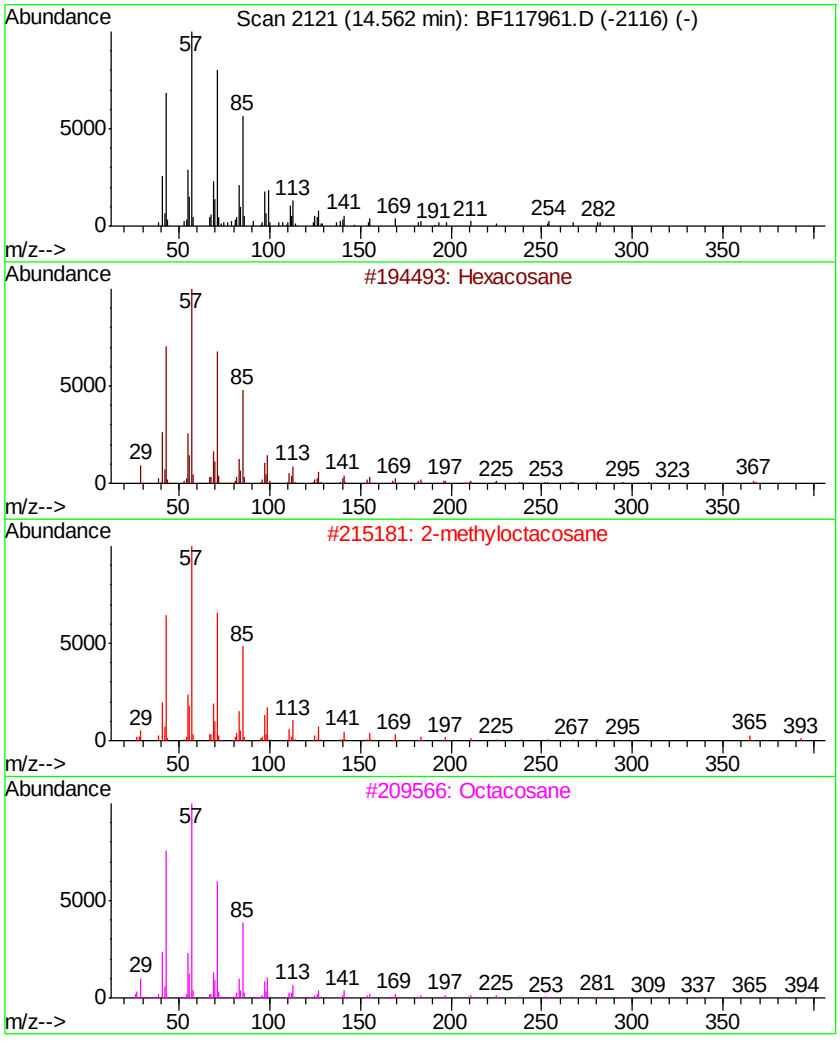
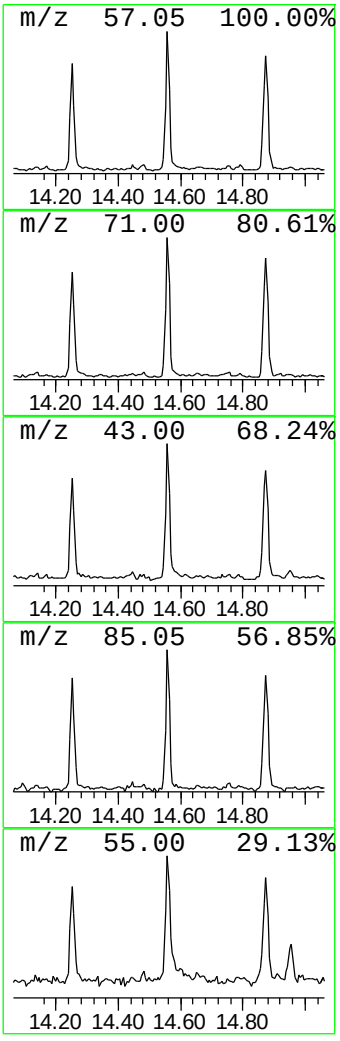
Peak Number 8 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	2.72 ng	192087	Chrysene-d12	14.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





Library Search Compound Report

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Data File : BF117961.D
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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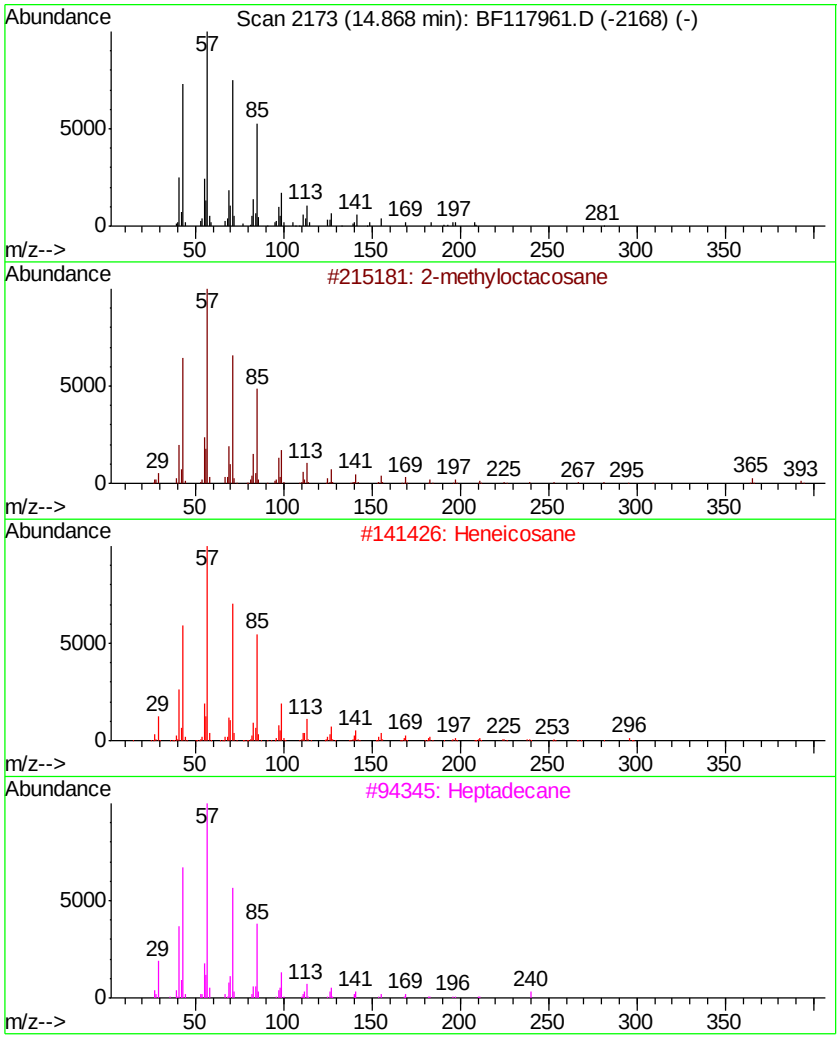
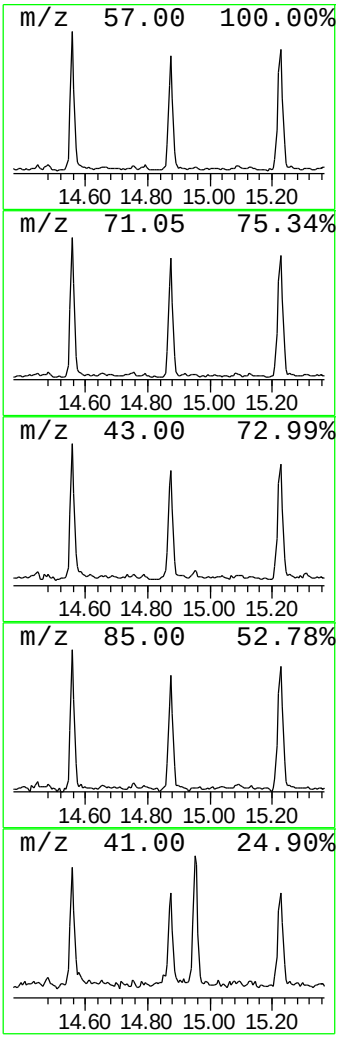
Peak Number 9 2-methyloctacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	3.16 ng	165154	Perylene-d12	15.60

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	240	C17H36	000629-78-7	91
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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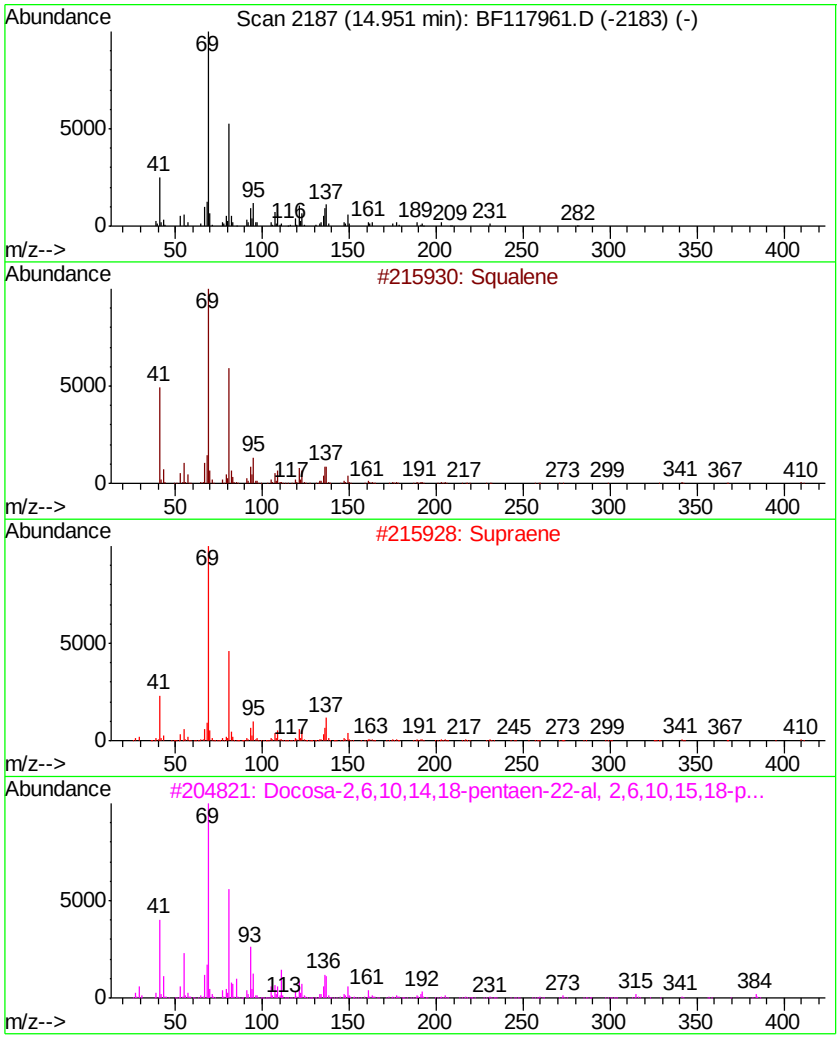
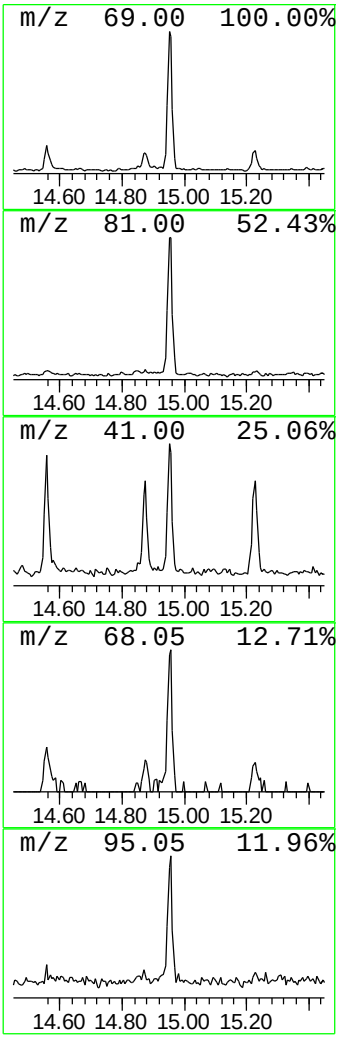
Peak Number 10 Squalene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	2.79 ng	145671	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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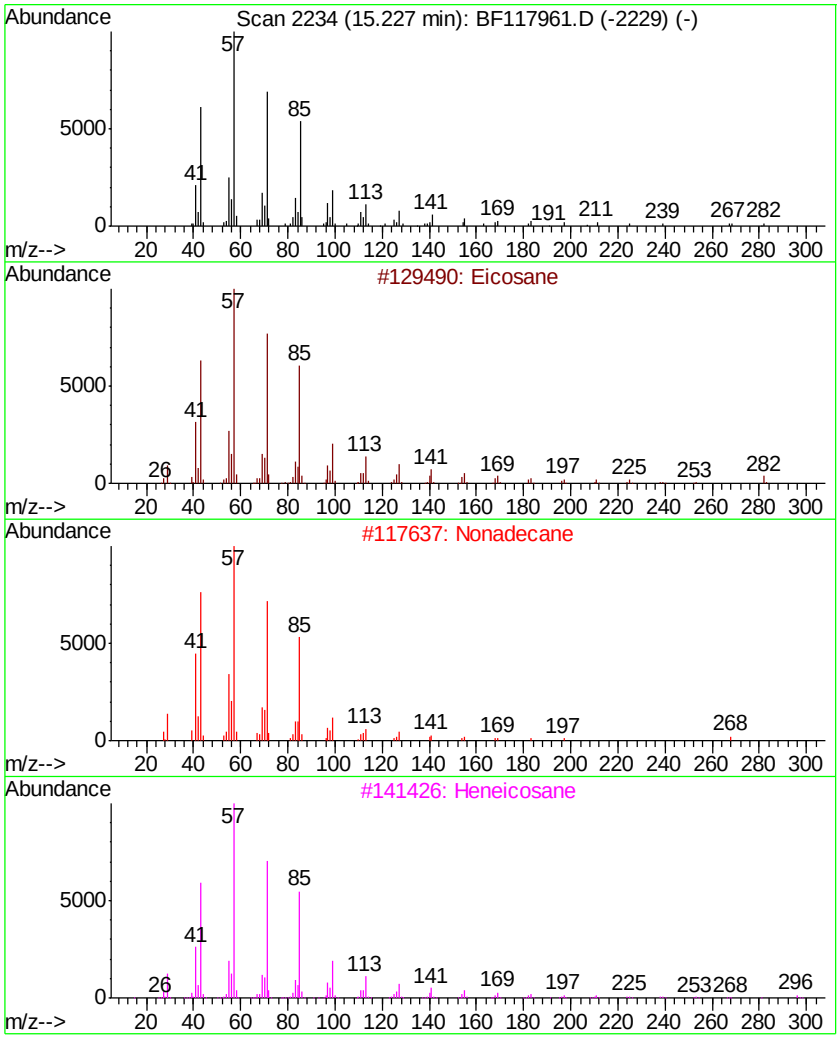
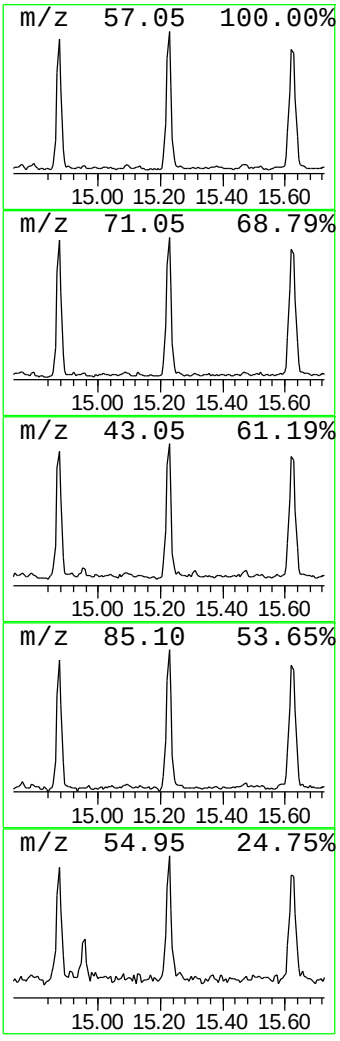
Peak Number 11 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.23	3.58 ng	187066	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Nonadecane	268	C19H40	000629-92-5	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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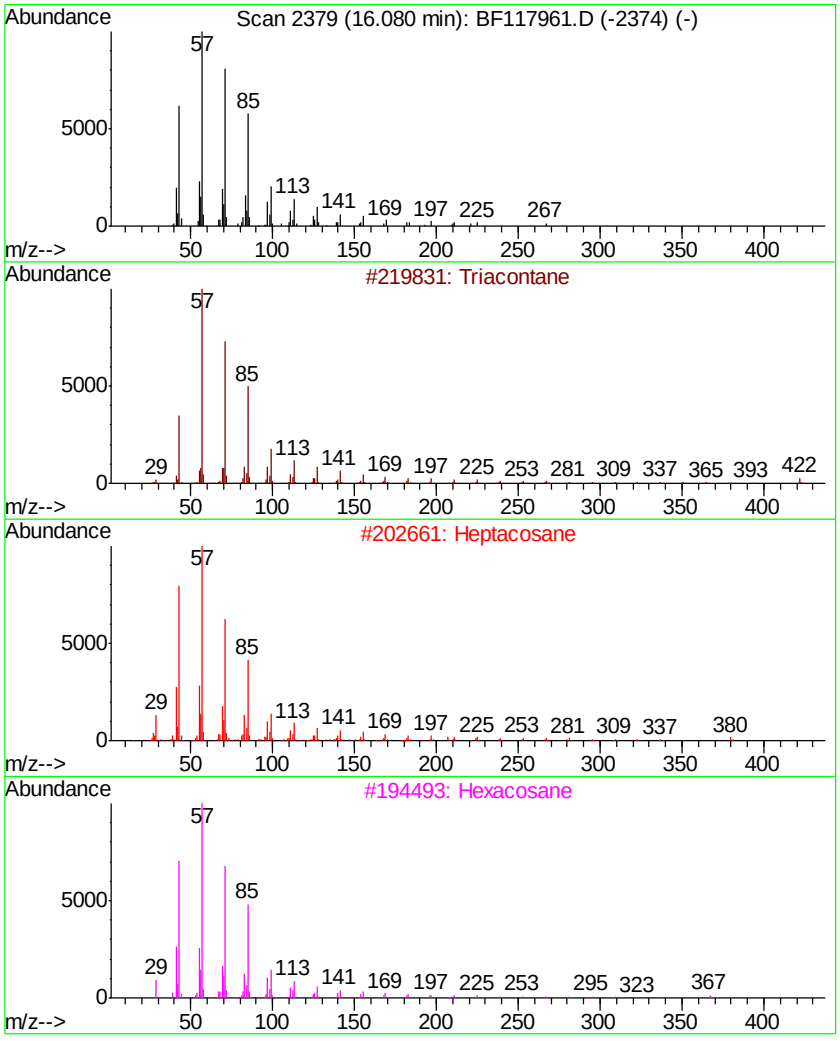
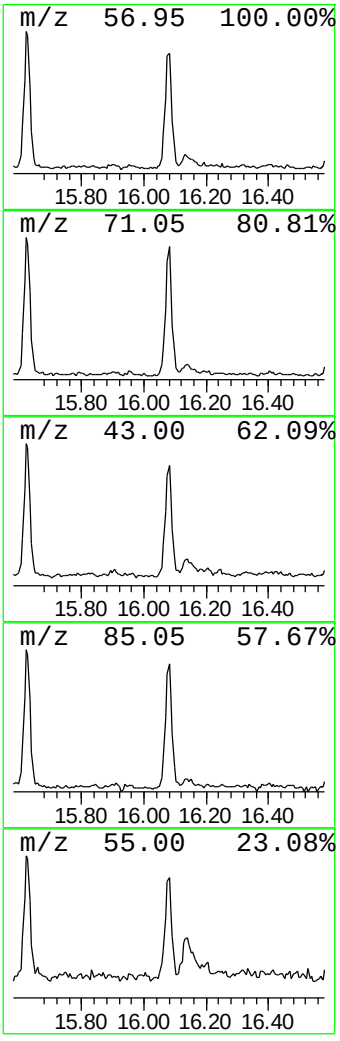
Peak Number 12 Triacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.08	3.32 ng	173240	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triacontane	422	C30H62	000638-68-6	91
2	Heptacosane	380	C27H56	000593-49-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Octacosane	394	C28H58	000630-02-4	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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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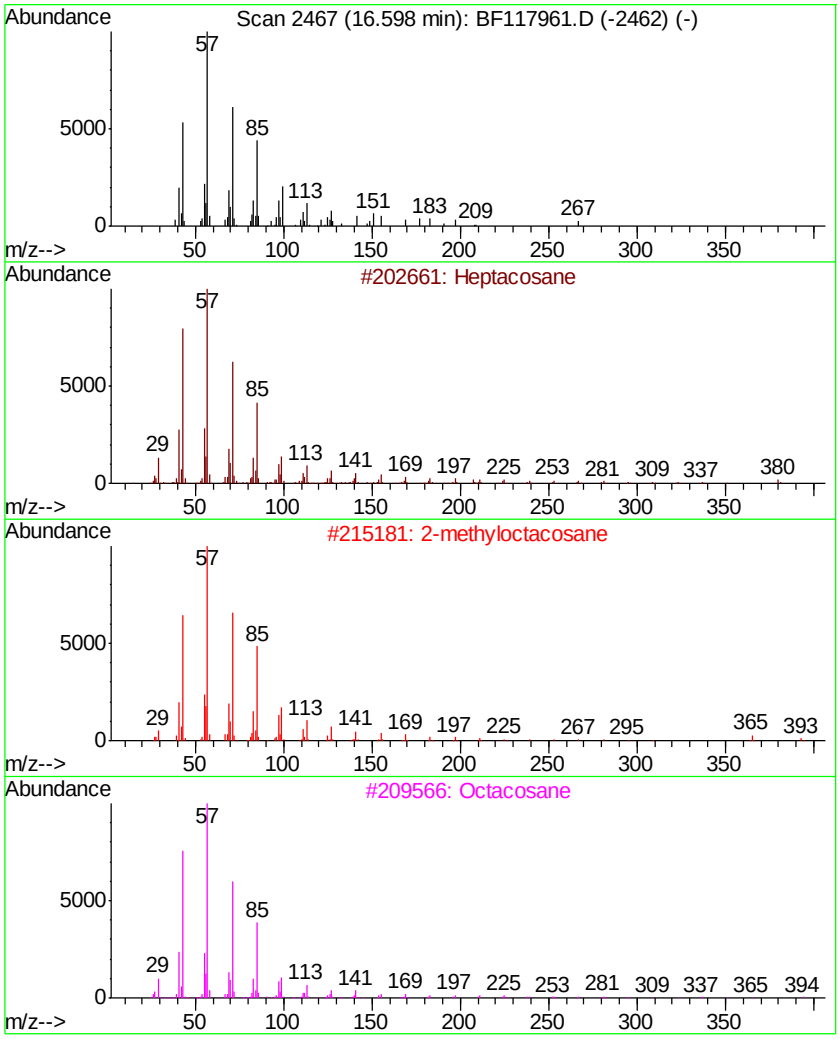
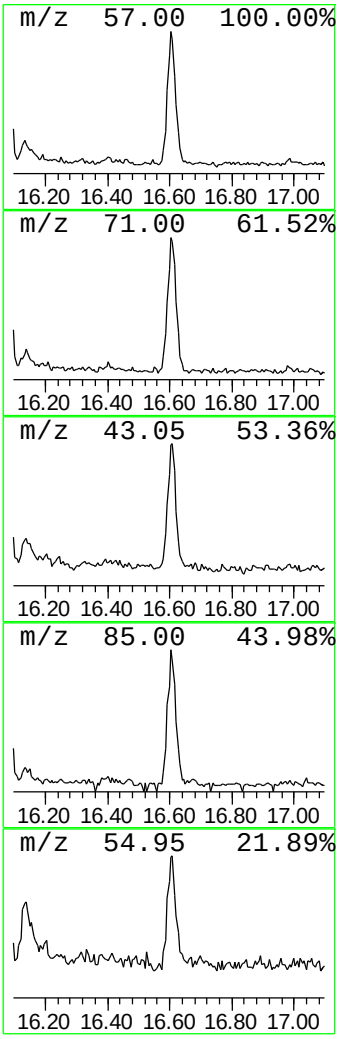
Peak Number 13 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	2.85 ng	148910	Perylene-d12	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Hentriacontane	437	C31H64	000630-04-6	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112319\
Data File : BF117961.D
Acq On : 23 Nov 2019 17:21
Operator : JU
Sample : K5951-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IRONBOUND-4FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.17	23.3	ng	943260	1	6.90	810069	20.0
2-Pentanone, 4-hy...	5.12	16.1	ng	650348	1	6.90	810069	20.0
unknown6.67	6.67	88.3	ng	3576600	1	6.90	810069	20.0
n-Hexadecanoic acid	11.97	9.0	ng	627697	4	11.45	1397210	20.0
Octadecanoic acid	12.75	3.2	ng	221244	4	11.45	1397210	20.0
1-Heneicosanol	13.93	7.2	ng	509771	5	14.09	1410590	20.0
Hexacosane	14.56	2.7	ng	192087	5	14.09	1410590	20.0
2-methyloctacosane	14.87	3.2	ng	165154	6	15.60	1044550	20.0
Squalene	14.95	2.8	ng	145671	6	15.60	1044550	20.0
Eicosane	15.23	3.6	ng	187066	6	15.60	1044550	20.0
Triacontane	16.08	3.3	ng	173240	6	15.60	1044550	20.0
Heptacosane	16.60	2.9	ng	148910	6	15.60	1044550	20.0