LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118608.D
Acq On : 20 Jan 2020 23:12
Operator : CG/JU
Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

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-BF012020.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	2.222	15	23	30	rBV	2760693	3979334	24.35%	2.848%
2	5.110	506	514	524	rBV	1991564	2863665	17.52%	2.050%
3	5.510	575	582	585	rBV	11016765	12578308	76.95%	9.003%
4	6.510	745	752	756	rBV	11253580	13903251	85.06%	9.952%
5	6.651	771	776	780	rBV	11909192	13746753	84.10%	9.840%
6	6.880	811	815	818	rBV	3425007	2975018	18.20%	2.129%
7	7.039	837	842	845	rBV	11303336	10818486	66.19%	7.744%
8	7.439	904	910	913	rBV	8031454	8742972	53.49%	6.258%
9	8.163	1028	1033	1036	rBV	3797888	3836059	23.47%	2.746%
10	9.239	1210	1216	1219	rBV	14881395	16345448	100.00%	11.700%
11	9.627	1277	1282	1285	rBV	1128623	907550	5.55%	0.650%
12	9.916	1325	1331	1335	rBV	5412265	4729281	28.93%	3.385%
13	10.704	1459	1465	1468	rBV	10414617	10898951	66.68%	7.801%
14	11.398	1579	1583	1587	rBV	4713744	4429198	27.10%	3.170%
15	11.927	1669	1673	1685	rBV	895794	920149	5.63%	0.659%
16	12.710	1803	1806	1819	rBV	279453	368879	2.26%	0.264%
17	12.992	1848	1854	1857	rBV	13536710	14544895	88.98%	10.411%
18	13.880	2002	2005	2014	rBV	1963934	1946947	11.91%	1.394%
19	14.033	2027	2031	2035	rBV	3029752	2729402	16.70%	1.954%
20	14.209	2057	2061	2066	rBV	394154	398455	2.44%	0.285%
21	14.515	2109	2113	2119	rBV	752107	719506	4.40%	0.515%
22	14.821	2161	2165	2174	rVB	724960	823924	5.04%	0.590%
23	14.903	2175	2179	2184	rVB	193701	214212	1.31%	0.153%
24	15.162	2219	2223	2232	rVB	672167	878645	5.38%	0.629%
25	15.503	2276	2281	2285	rBV	2211351	2799241	17.13%	2.004%
26	15.551	2285	2289	2298	rVB	612329	849998	5.20%	0.608%
27	15.998	2359	2365	2369	rBV	420615	694289	4.25%	0.497%
28	16.039	2369	2372	2382	rVB	222576	354945	2.17%	0.254%
29	16.509	2446	2452	2460	rVB2	218855	406408	2.49%	0.291%
30	17.192	2562	2568	2577	rBV5	141405	301970	1.85%	0.216%

Sum of corrected areas: 139706139

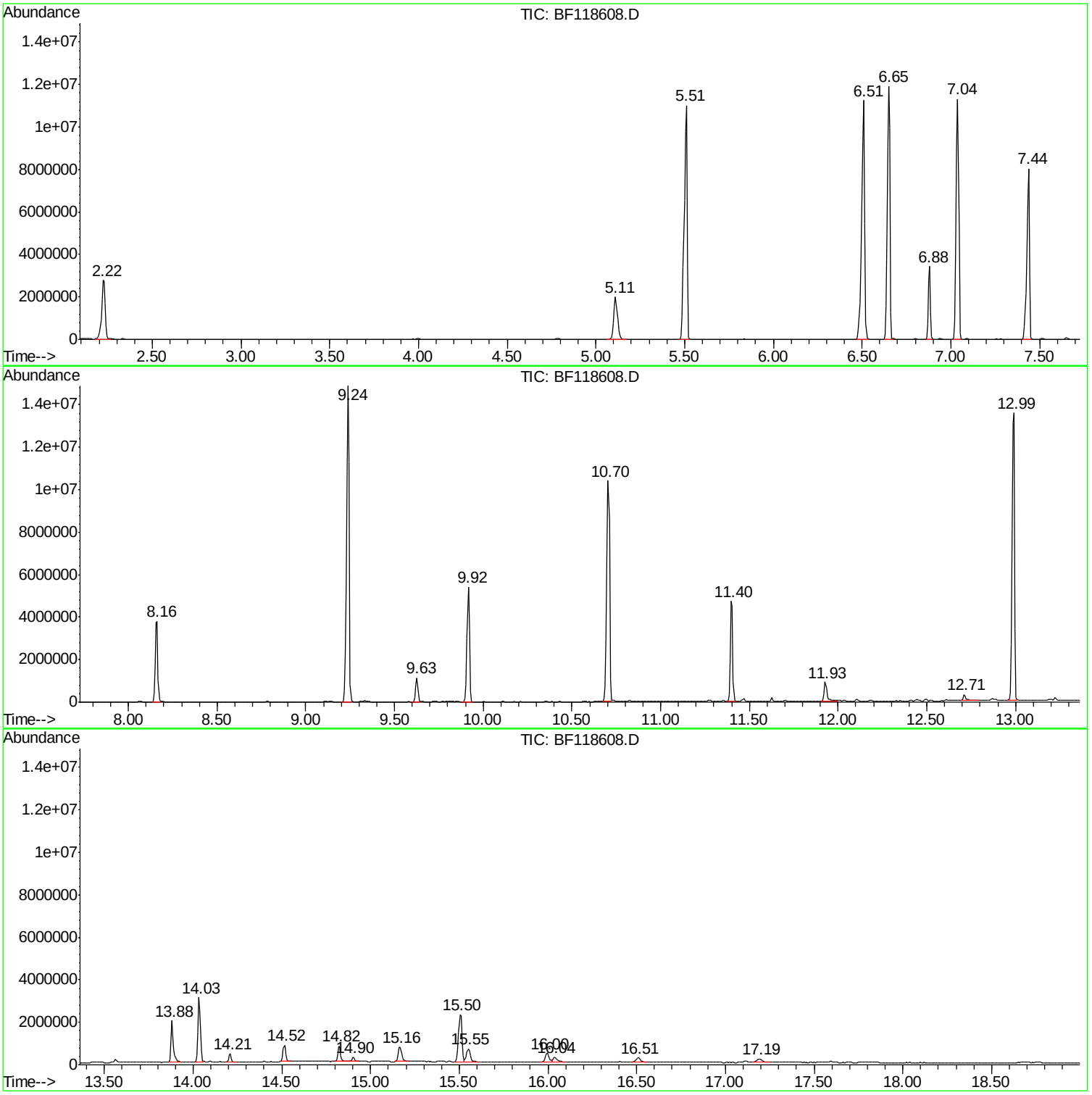
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118608.D
Acq On : 20 Jan 2020 23:12
Operator : CG/JU
Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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\BF012020\
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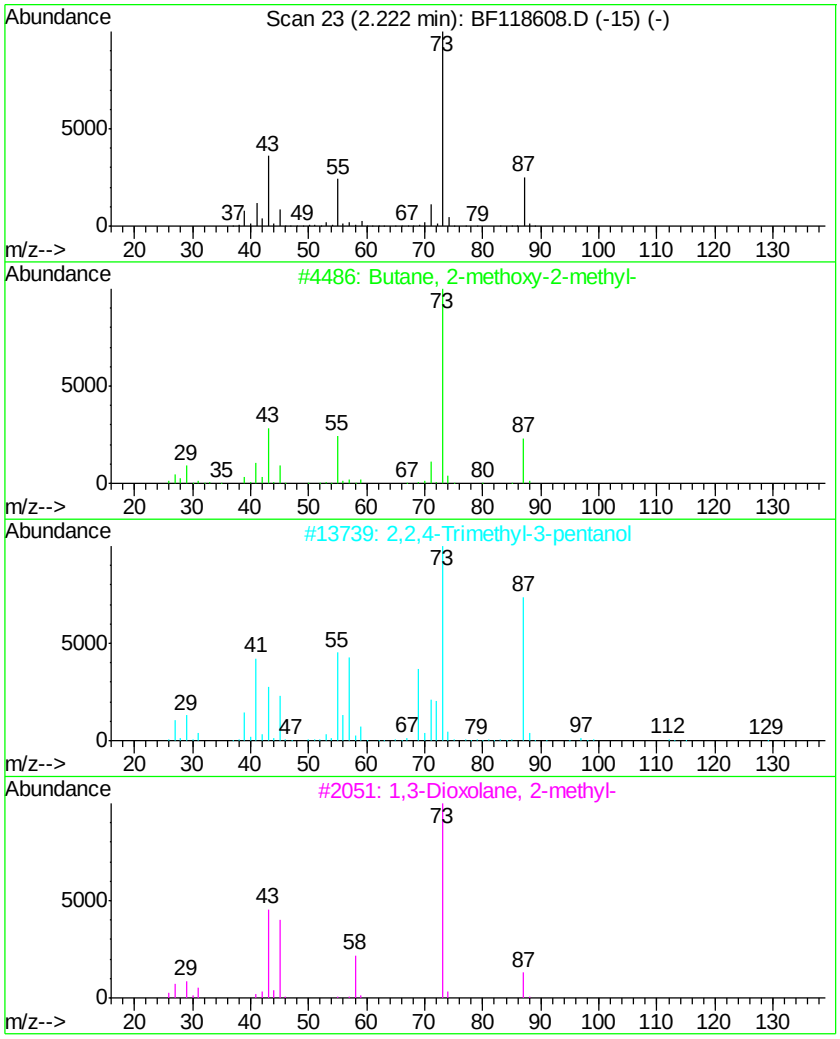
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

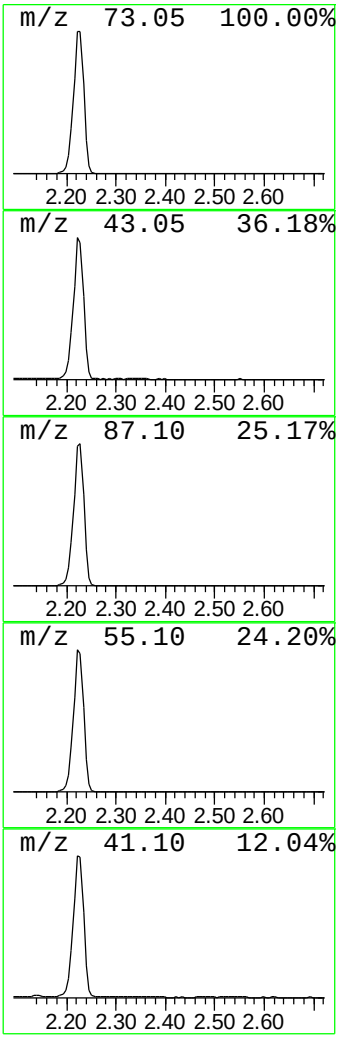
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	26.75 ng	3979330	1,4-Dichlorobenzene-d4	6.88

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	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22





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Data File : BF118608.D
Acq On : 20 Jan 2020 23:12
Operator : CG/JU
Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

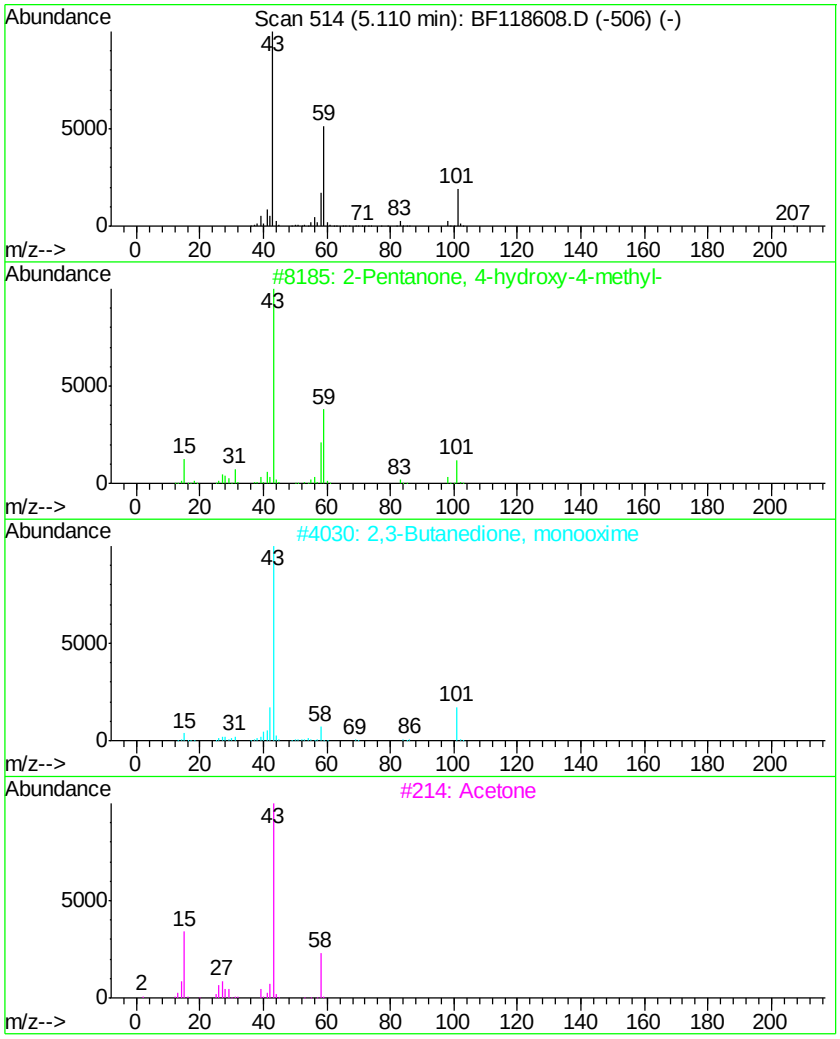
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

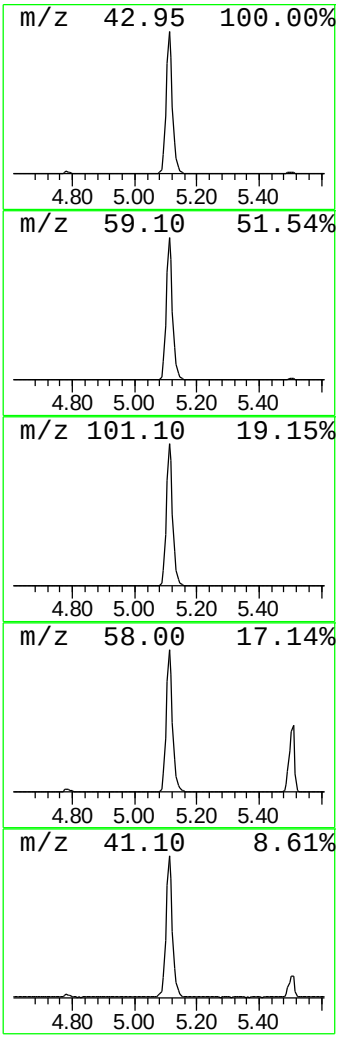
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	19.25 ng	2863670	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
3	Acetone	58	C3H6O	000067-64-1	10
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

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Operator : CG/JU
Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

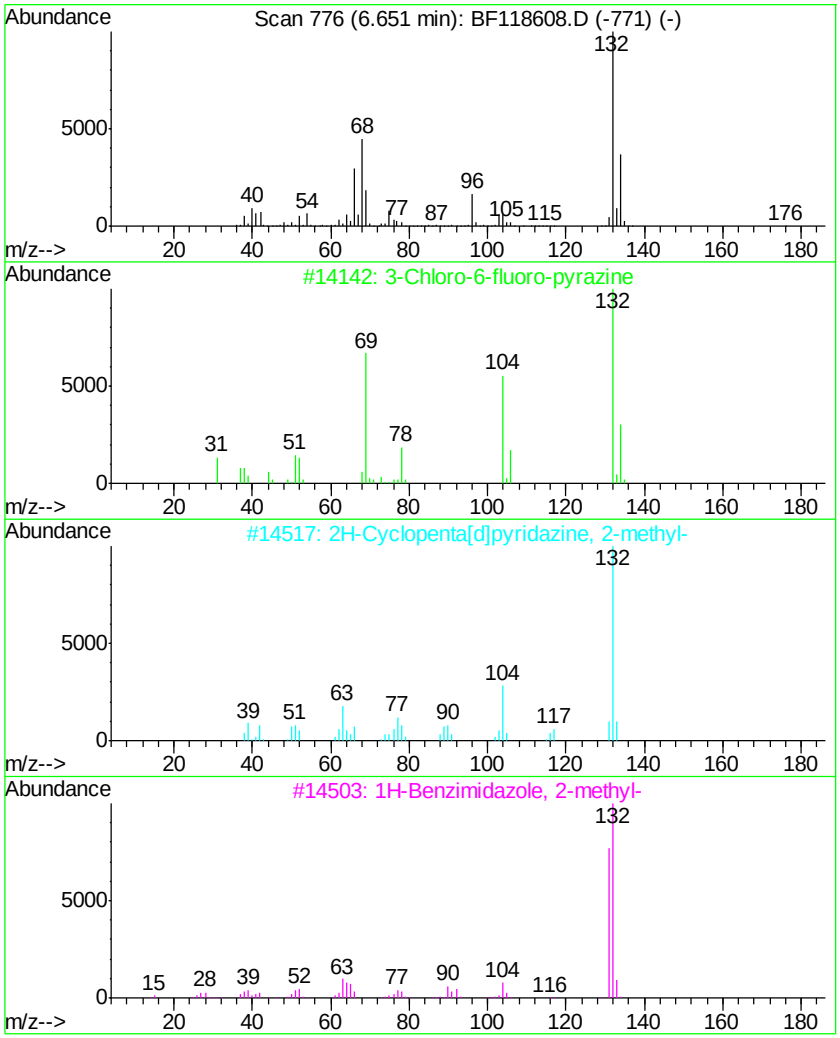
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

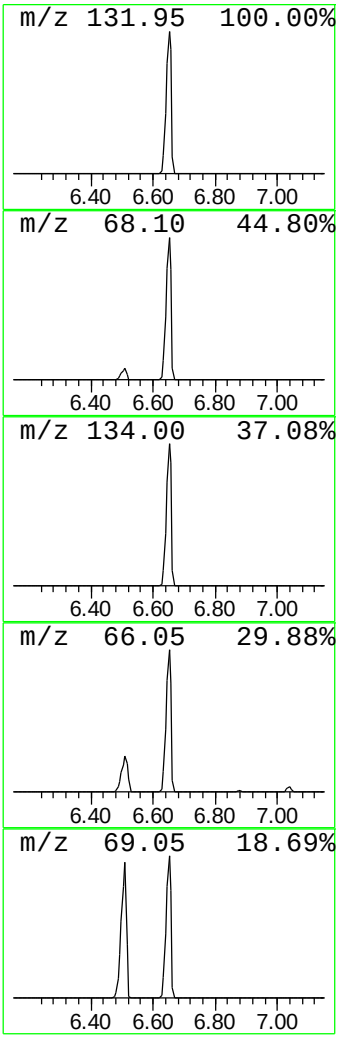
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	92.41 ng	13746800	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
5	1-Isoquinolinemethanol, .alpha.-...	191	C12H17NO	114608-92-3	12





Library Search Compound Report

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Data File : BF118608.D
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Operator : CG/JU
Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

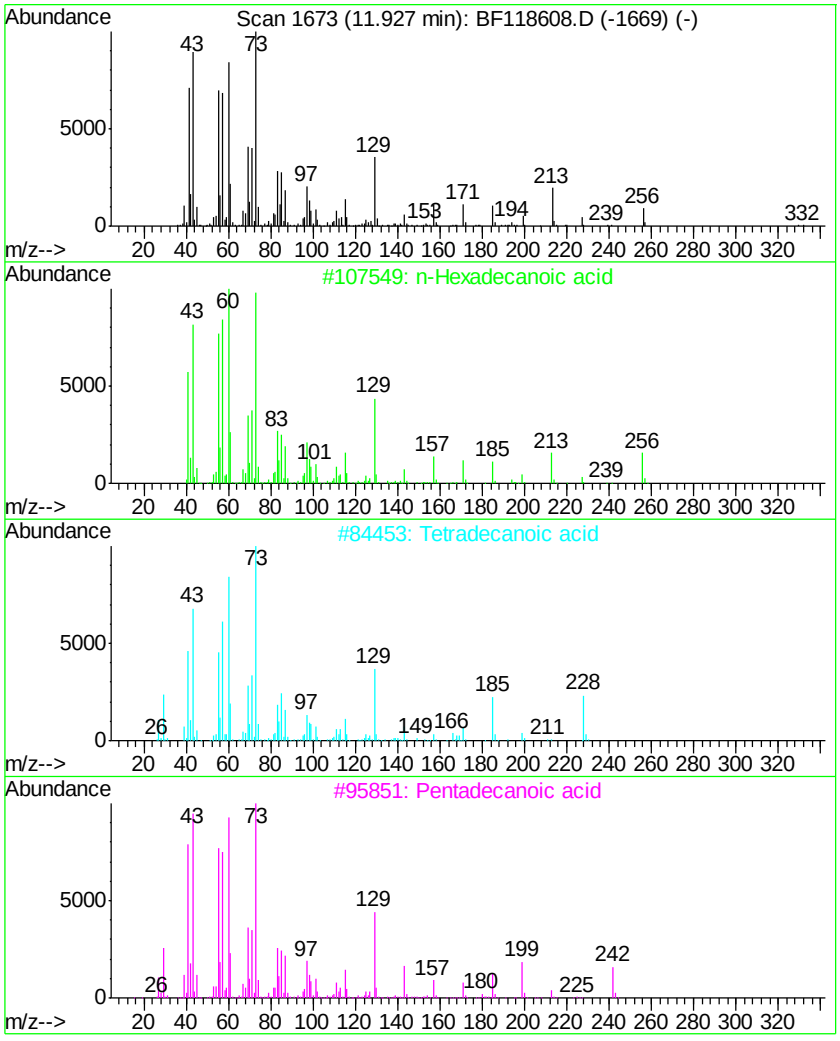
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

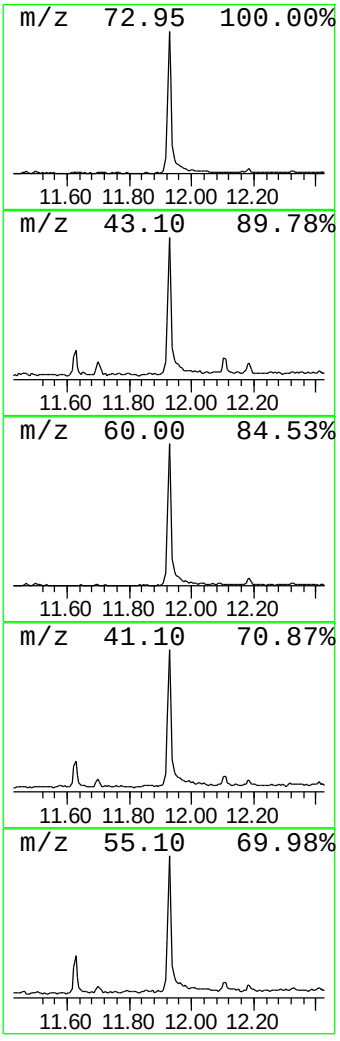
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	4.15 ng	920149	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Octadecanoic acid	284	C18H36O2	000057-11-4	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	81





Library Search Compound Report

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Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

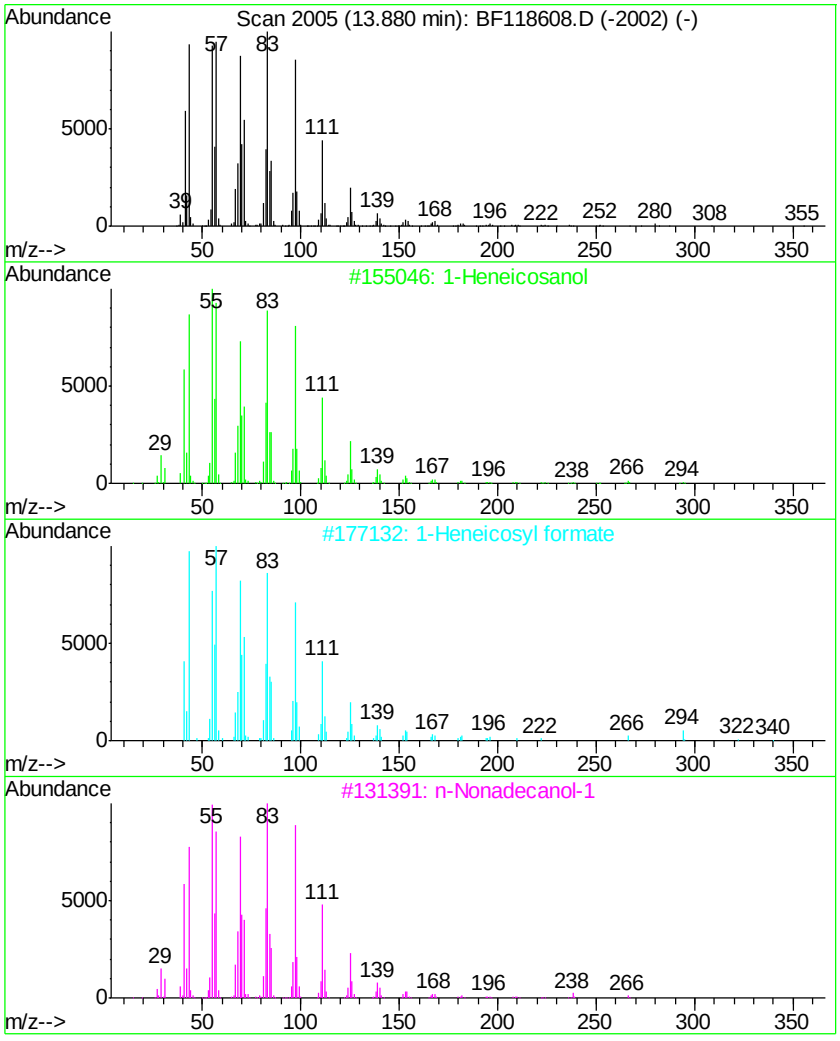
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

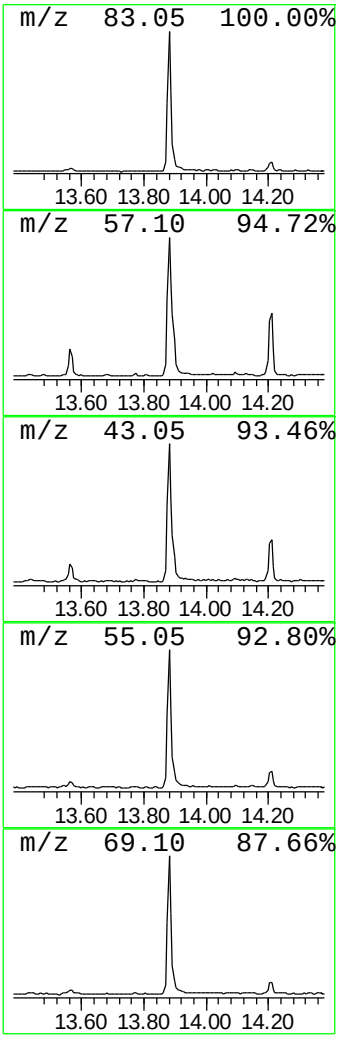
****

Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	14.27 ng	1946950	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93





Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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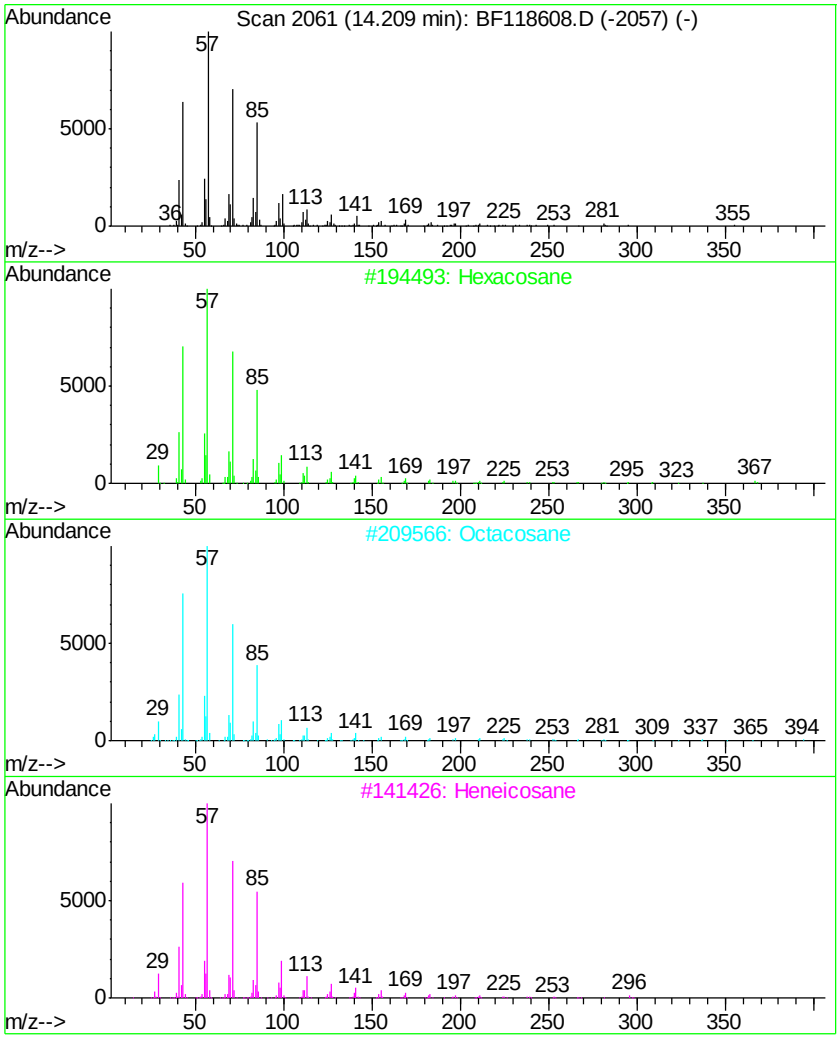
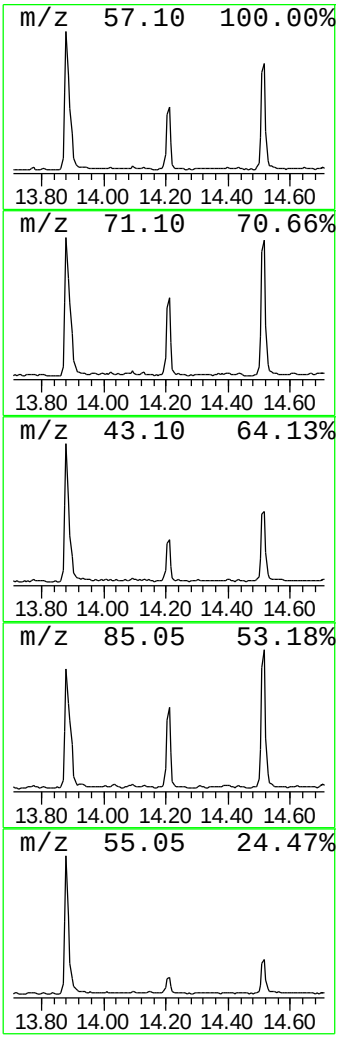
****

Peak Number 7 Hexacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.21	2.92 ng	398455	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

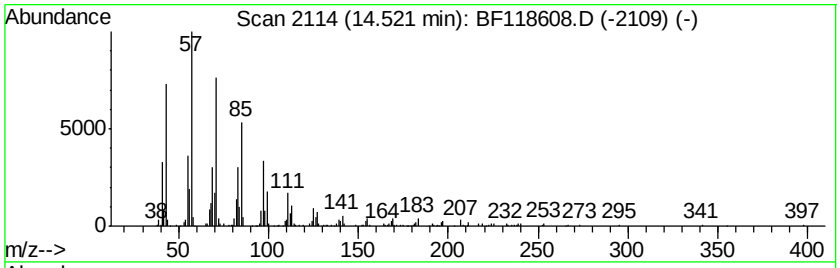
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

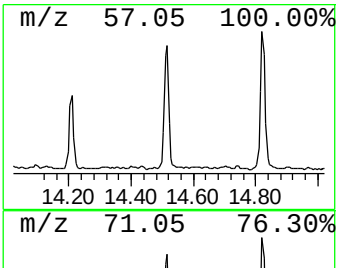
****

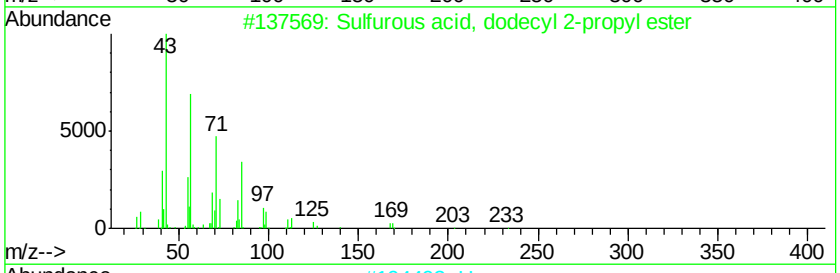
Peak Number 8 Sulfurous acid, dodecyl 2-p... Concentration Rank 8

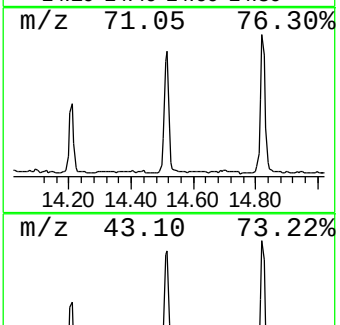
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	5.27 ng	719506	Chrysene-d12	14.03

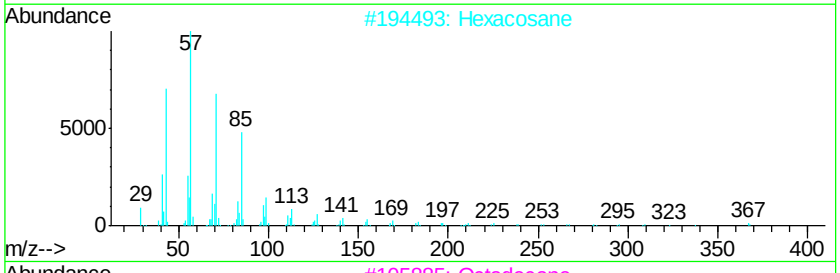
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	91
2	Hexacosane	366	C26H54	000630-01-3	83
3	Octadecane	254	C18H38	000593-45-3	76
4	Octacosane	394	C28H58	000630-02-4	74
5	Hexadecane	226	C16H34	000544-76-3	68

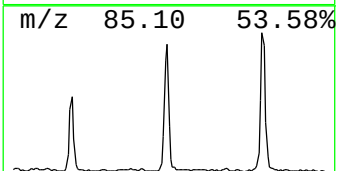


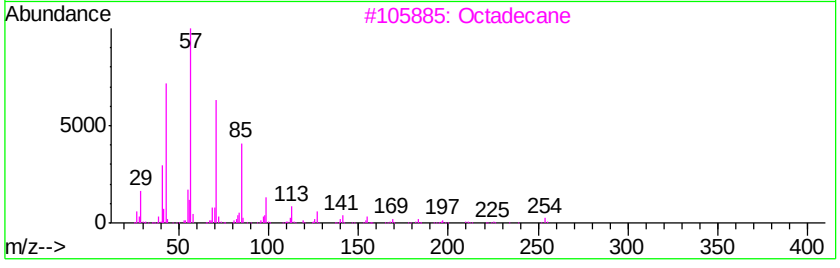












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Instrument : BNA_F
ClientSampleId : EP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

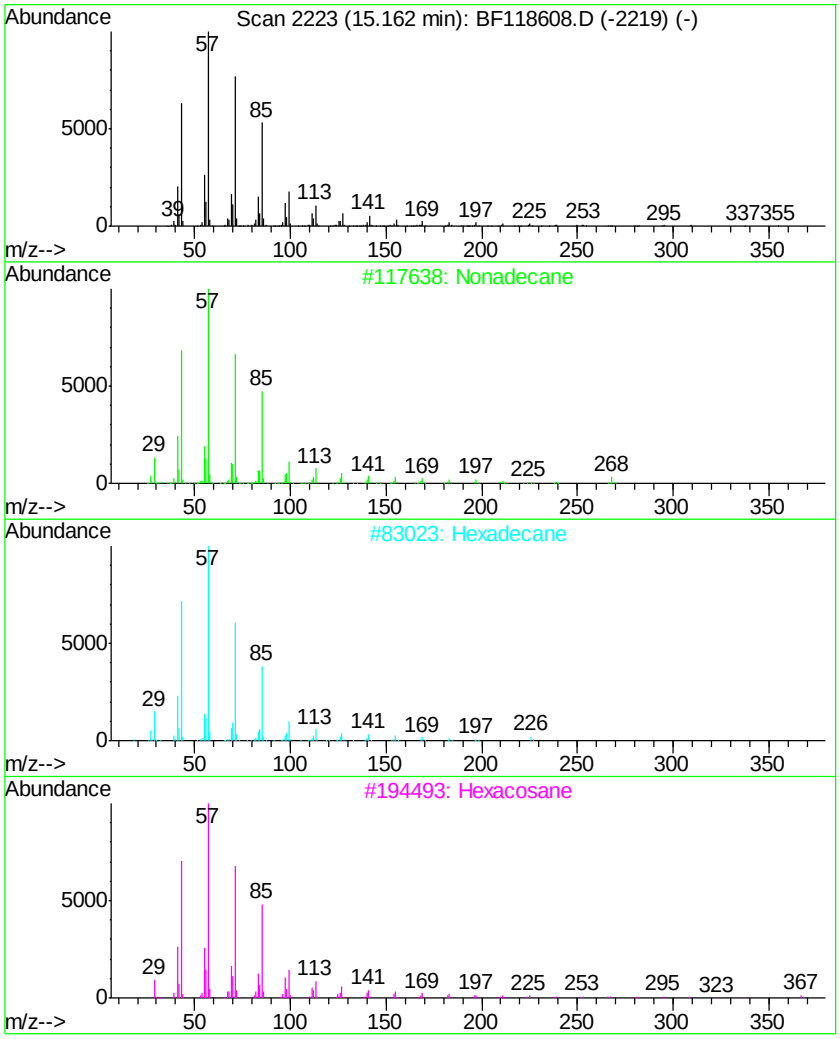
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

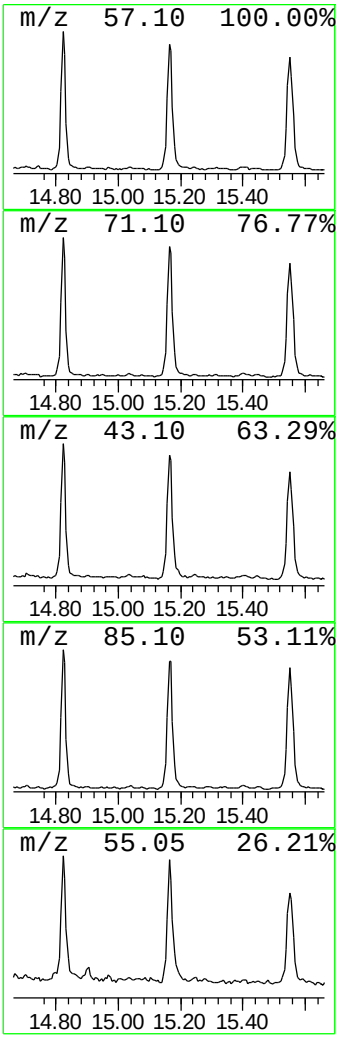
****

Peak Number 10 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	6.28 ng	878645	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	95
2	Hexadecane	226	C16H34	000544-76-3	95
3	Hexacosane	366	C26H54	000630-01-3	94
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Sample : L1176-10
Misc :
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Instrument : BNA_F
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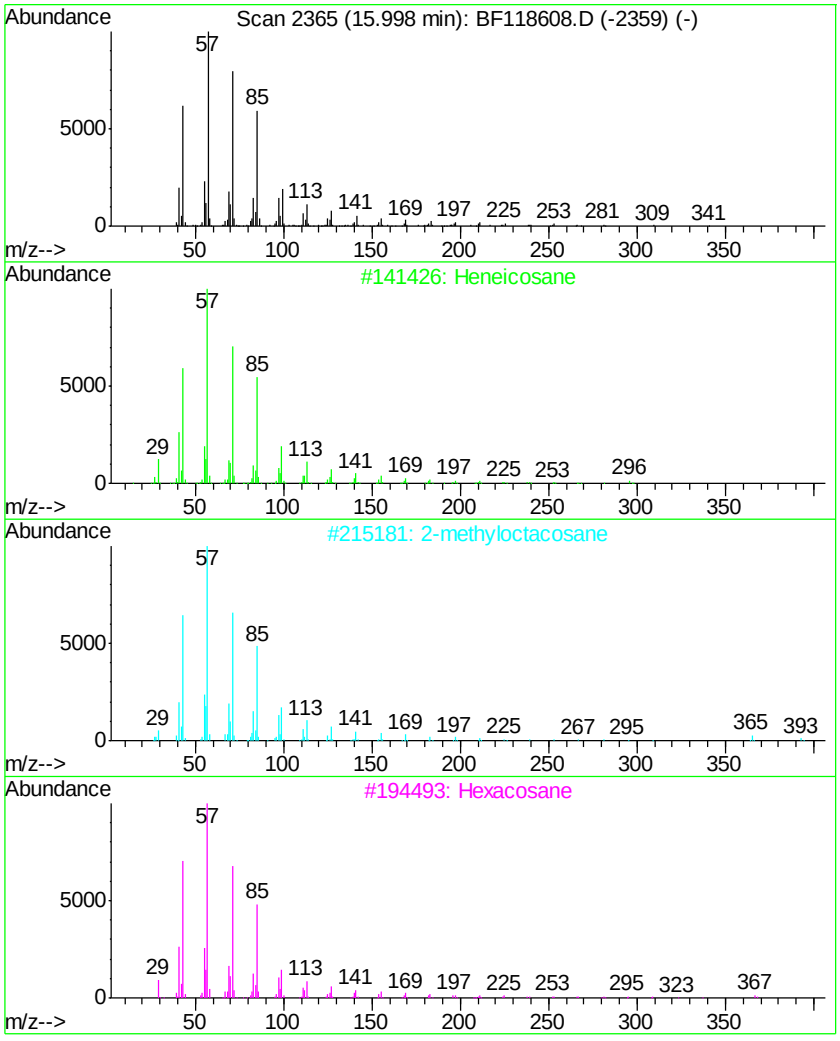
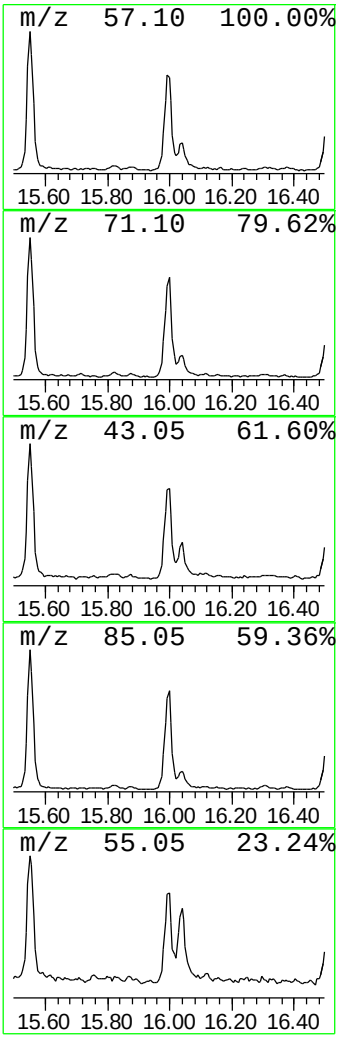
****

Peak Number 11 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.00	4.96 ng	694289	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hexacosane	366	C26H54	000630-01-3	90
4	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
5	Octadecane	254	C18H38	000593-45-3	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118608.D
Acq On : 20 Jan 2020 23:12
Operator : CG/JU
Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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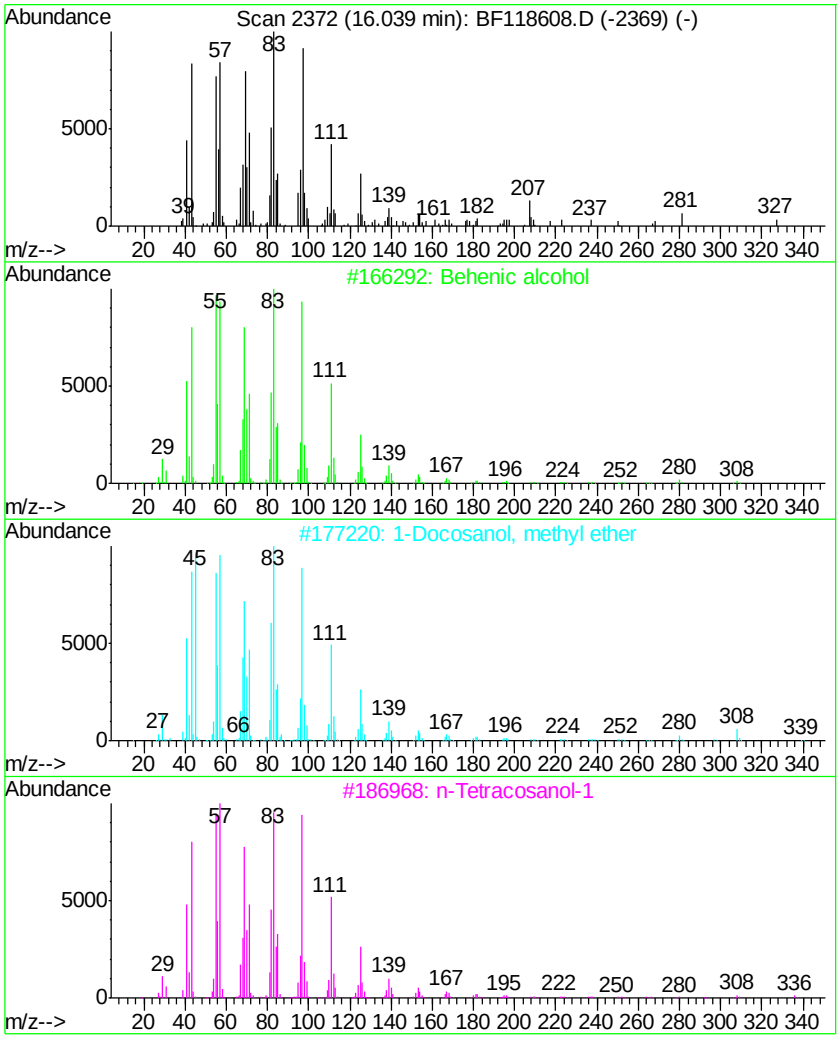
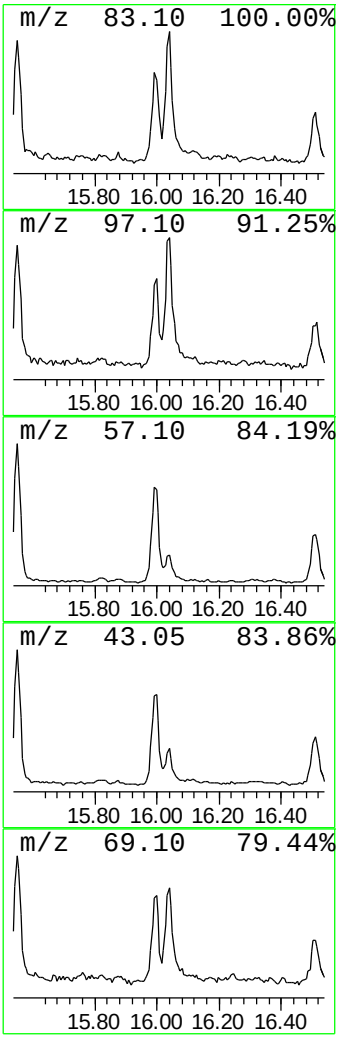
Peak Number 12 Behenic alcohol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	2.54 ng	354945	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	91
2	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	81
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	81
4	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	74
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118608.D
Acq On : 20 Jan 2020 23:12
Operator : CG/JU
Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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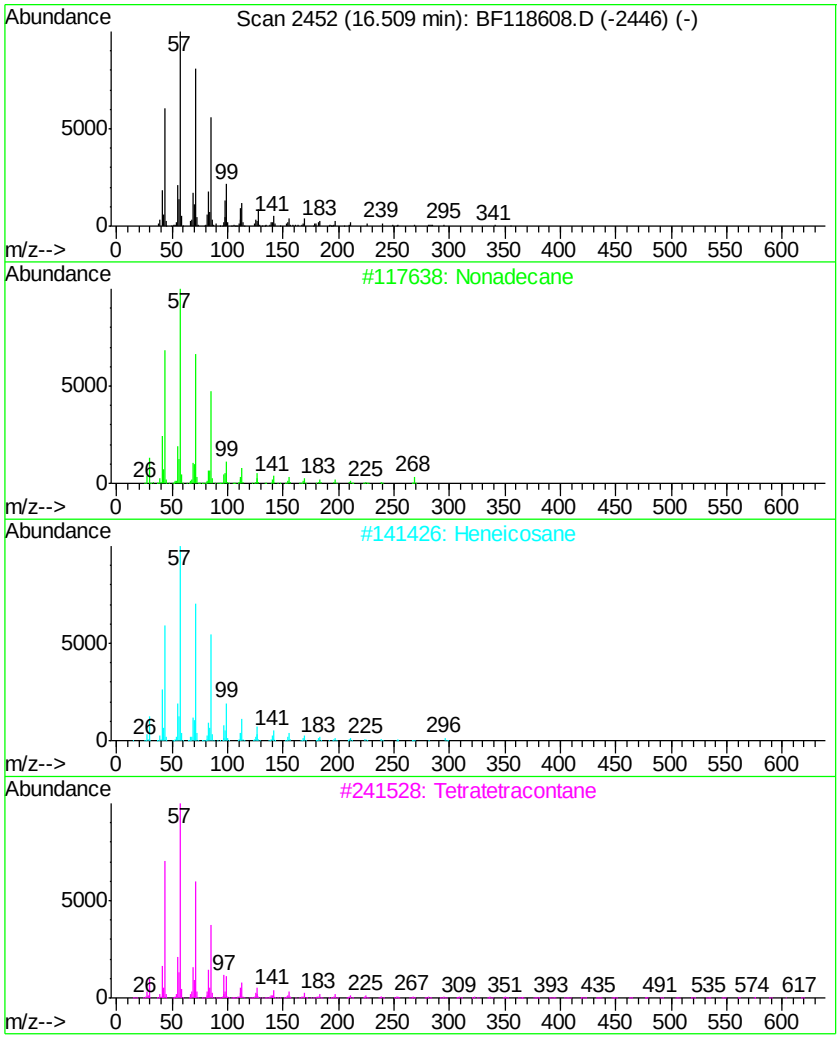
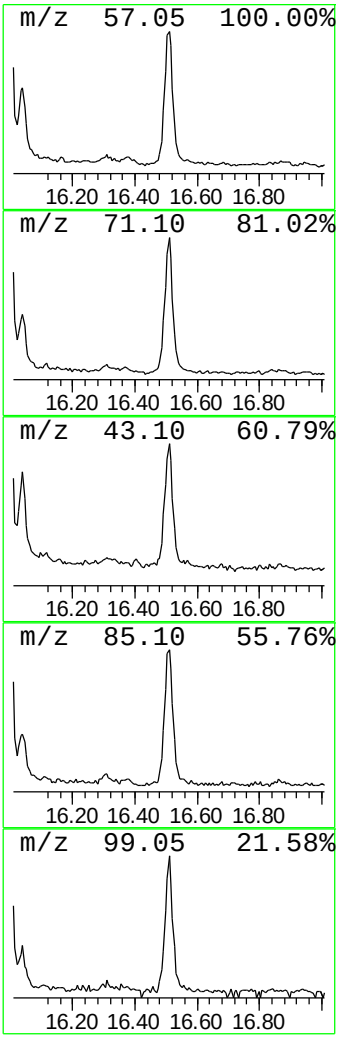
Peak Number 13 Tetratetracontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.51	2.90 ng	406408	Perylene-d12	15.51

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	Tetratetracontane	619	C44H90	007098-22-8	91
4	Octacosane	394	C28H58	000630-02-4	91
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF012020\
Data File : BF118608.D
Acq On : 20 Jan 2020 23:12
Operator : CG/JU
Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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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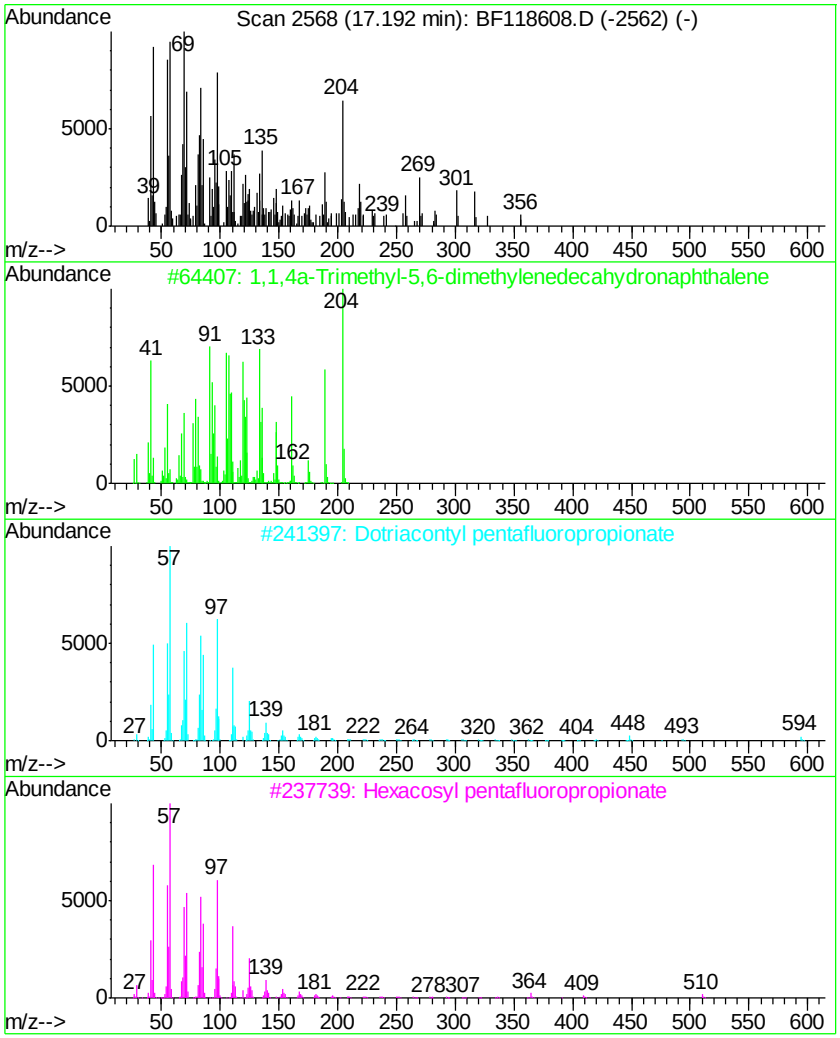
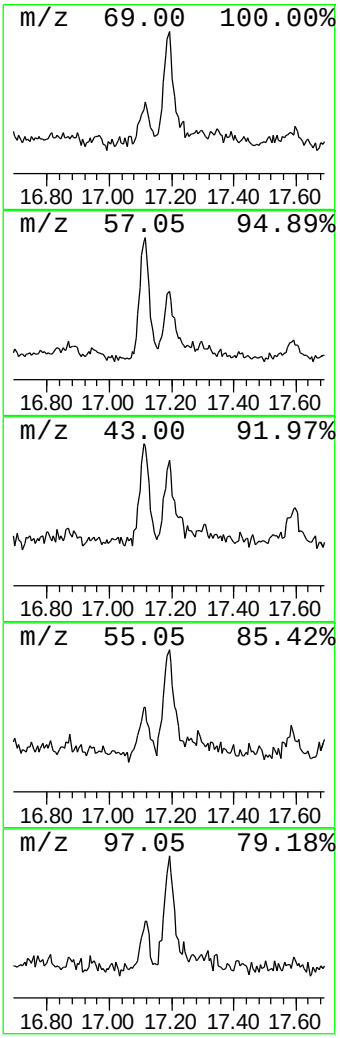
Peak Number 14 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.19	2.16 ng	301970	Perylene-d12	15.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	56
2	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	35
3	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	35
4	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	35
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF012020\
Data File : BF118608.D
Acq On : 20 Jan 2020 23:12
Operator : CG/JU
Sample : L1176-10
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : EP-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF012020.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...	2.22	26.8	ng	3979330	1	6.88	2975020	20.0
2-Pentanone, 4-hy...	5.11	19.3	ng	2863670	1	6.88	2975020	20.0
unknown6.65	6.65	92.4	ng	13746800	1	6.88	2975020	20.0
n-Hexadecanoic acid	11.93	4.2	ng	920149	4	11.40	4429200	20.0
1-Heneicosanol	13.88	14.3	ng	1946950	5	14.03	2729400	20.0
Hexacosane	14.21	2.9	ng	398455	5	14.03	2729400	20.0
Sulfurous acid, d...	14.52	5.3	ng	719506	5	14.03	2729400	20.0
Nonadecane	15.16	6.3	ng	878645	6	15.51	2799240	20.0
Heneicosane	16.00	5.0	ng	694289	6	15.51	2799240	20.0
Behenic alcohol	16.04	2.5	ng	354945	6	15.51	2799240	20.0
Tetratetracontane	16.51	2.9	ng	406408	6	15.51	2799240	20.0
1,1,4a-Trimethyl-...	17.19	2.2	ng	301970	6	15.51	2799240	20.0