

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
 Data File : BF117659.D
 Acq On : 31 Oct 2019 15:44
 Operator : JU
 Sample : K5540-17
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 159-46-(0-1)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF101819.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	5.357	553	556	577	rBV	386086	631789	79.63%	9.602%
2	6.386	728	731	748	rBV	489985	753488	94.97%	11.452%
3	6.504	748	751	772	rVB	769433	793356	100.00%	12.058%
4	6.728	786	789	799	rVB	185305	175893	22.17%	2.673%
5	6.881	812	815	832	rBV	543380	498342	62.81%	7.574%
6	7.298	883	886	903	rBV	257094	421221	53.09%	6.402%
7	8.010	1004	1007	1028	rBV	133299	231627	29.20%	3.520%
8	9.080	1186	1189	1204	rBV	557218	630609	79.49%	9.585%
9	9.486	1255	1258	1274	rBB	54056	66971	8.44%	1.018%
10	9.763	1301	1305	1323	rBB	258397	279255	35.20%	4.244%
11	10.557	1437	1440	1455	rBV	320085	419502	52.88%	6.376%
12	11.251	1555	1558	1568	rBV	214638	281894	35.53%	4.284%
13	11.780	1644	1648	1656	rBV2	14832	23019	2.90%	0.350%
14	12.474	1763	1766	1772	rBV	22328	23583	2.97%	0.358%
15	12.704	1799	1805	1810	rBV	25129	27665	3.49%	0.420%
16	12.827	1822	1826	1835	rBV	606782	567194	71.49%	8.621%
17	13.727	1975	1979	1989	rBV2	57449	112293	14.15%	1.707%
18	13.898	2004	2008	2020	rVB	167709	211714	26.69%	3.218%
19	14.039	2029	2032	2035	rBV	7012	8984	1.13%	0.137%
20	14.339	2080	2083	2086	rBV	11931	12411	1.56%	0.189%
21	14.639	2129	2134	2139	rBV	21837	23399	2.95%	0.356%
22	14.951	2182	2187	2192	rVB3	29122	39216	4.94%	0.596%
23	15.227	2232	2234	2239	rVB5	5311	8076	1.02%	0.123%
24	15.304	2239	2247	2250	rBV3	26895	43814	5.52%	0.666%
25	15.339	2250	2253	2266	rVB	109442	172436	21.74%	2.621%
26	15.709	2311	2316	2324	rVB2	25420	44491	5.61%	0.676%
27	15.798	2326	2331	2336	rBV8	7384	18804	2.37%	0.286%
28	16.180	2391	2396	2401	rBV5	15634	28189	3.55%	0.428%
29	16.721	2483	2488	2499	rVB5	8490	21008	2.65%	0.319%
30	17.356	2590	2596	2599	rBV6	4528	9202	1.16%	0.140%

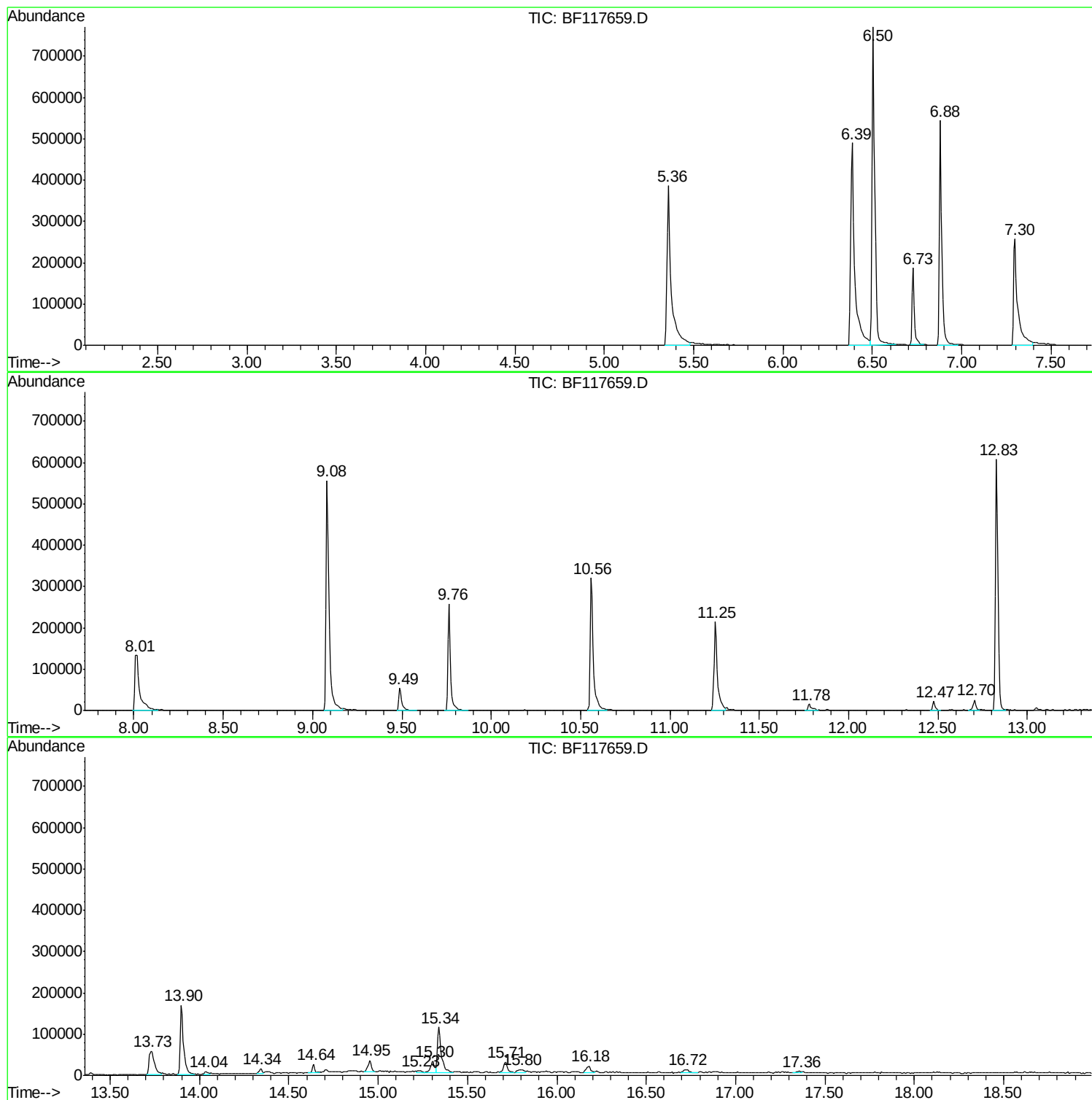
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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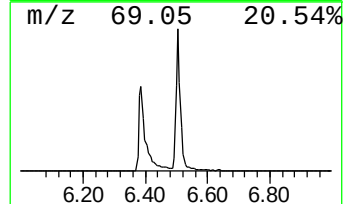
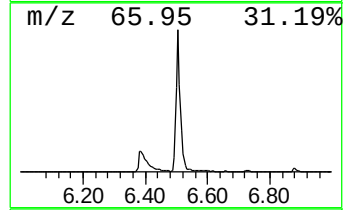
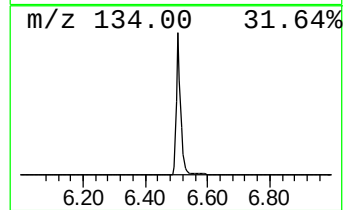
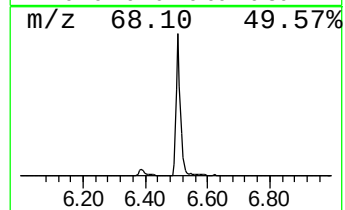
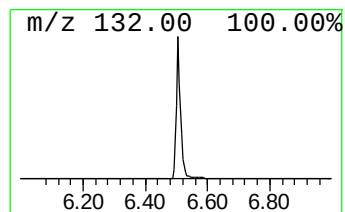
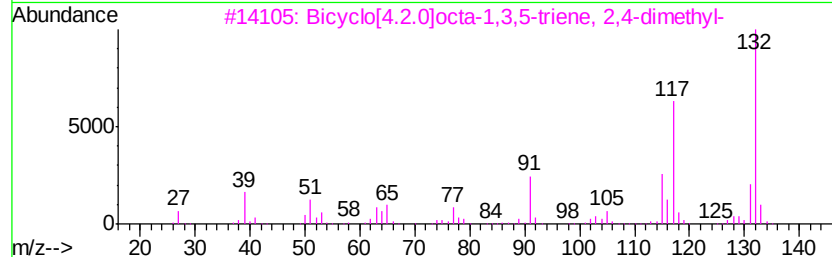
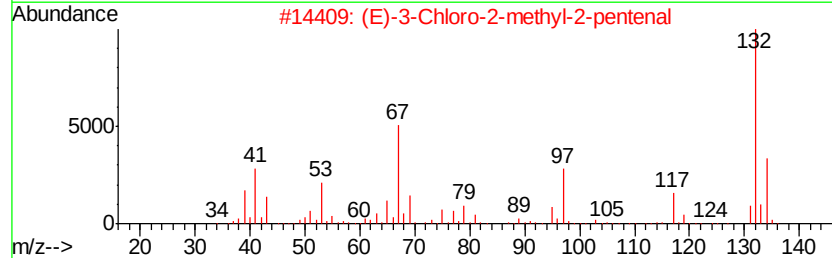
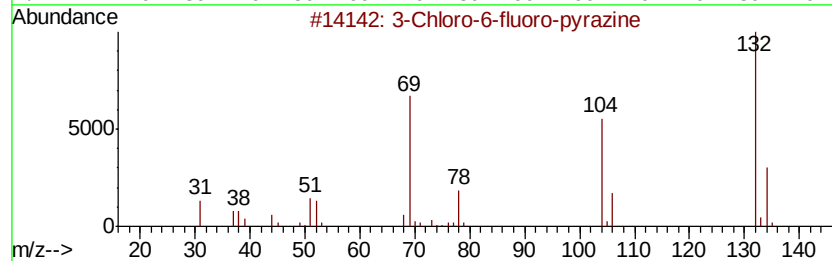
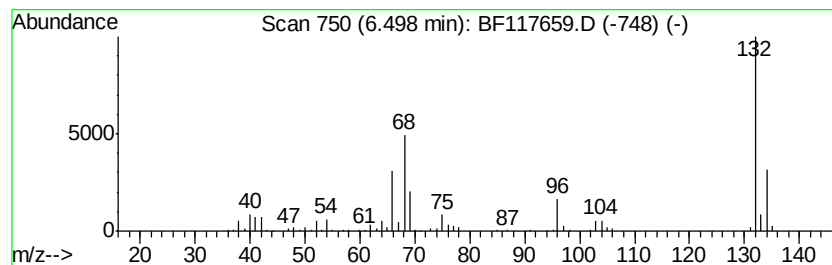
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	90.21 ng	793356	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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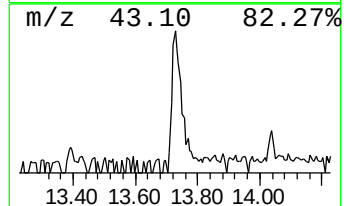
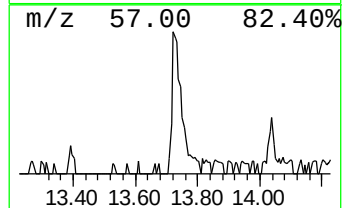
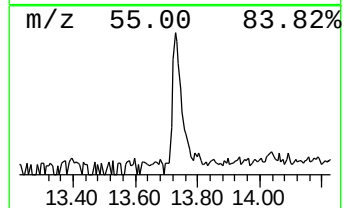
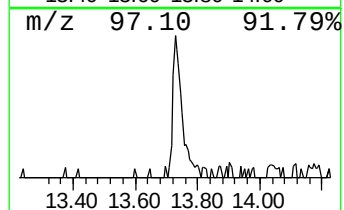
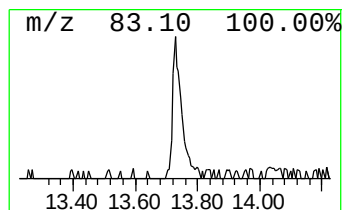
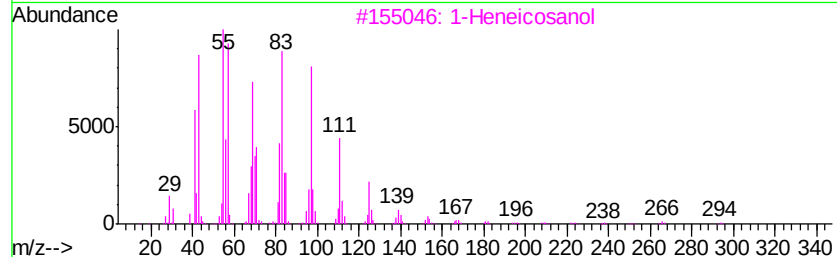
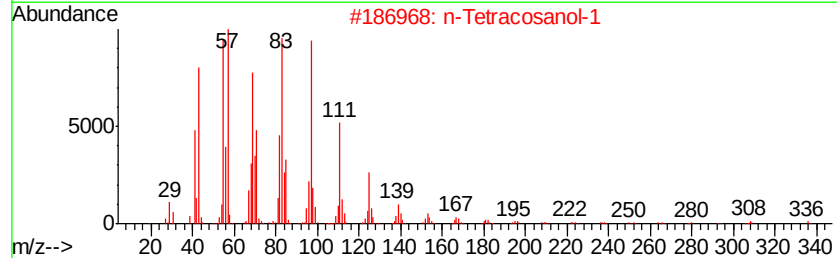
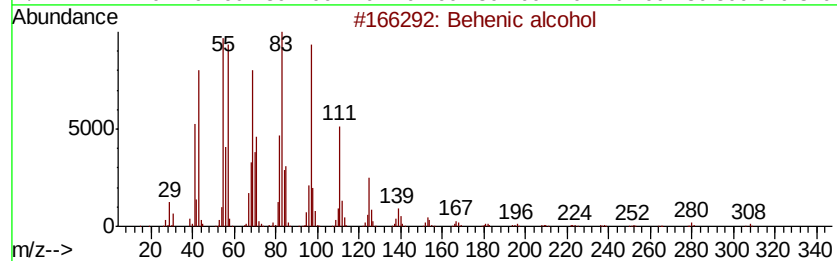
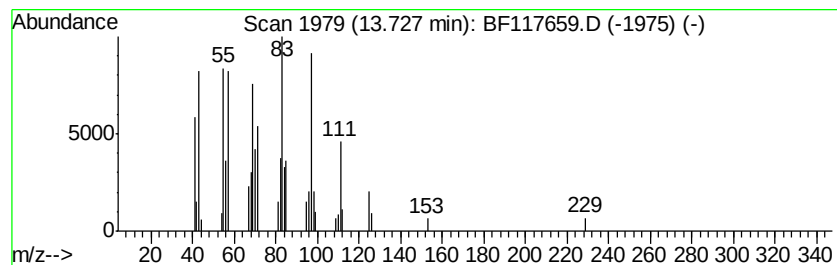
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	10.61 ng	112293	Chrysene-d12	13.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	95
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	91
4		1-Heptacosanol	396	C27H56O	002004-39-9	91
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	91



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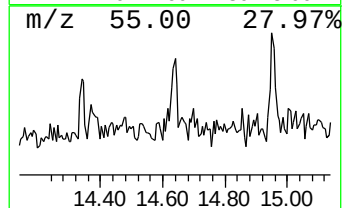
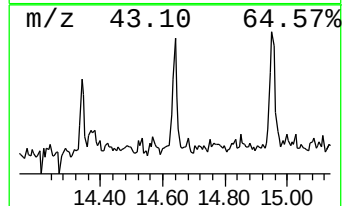
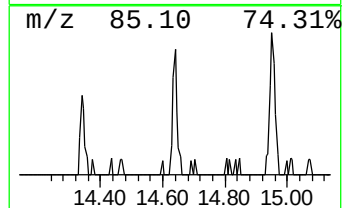
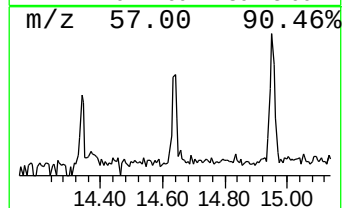
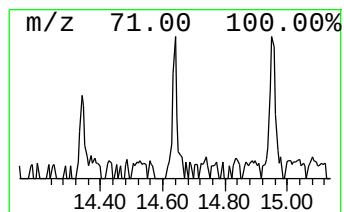
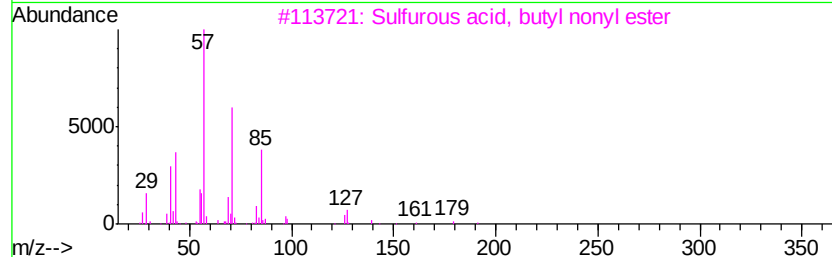
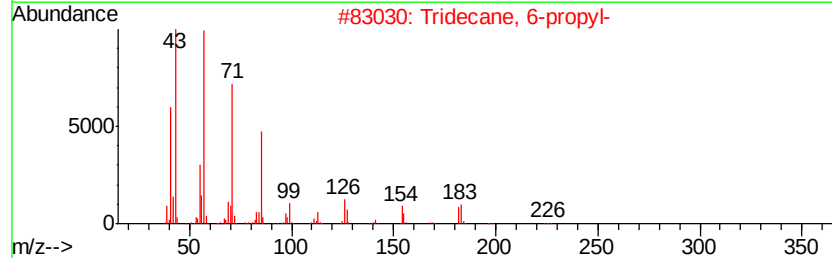
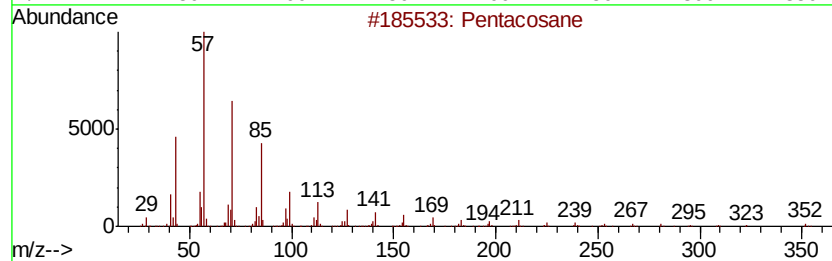
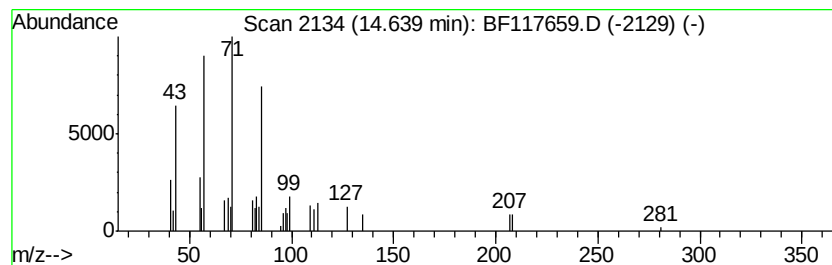
Instrument :
 BNA_F
 ClientSampled :
 159-46-(0-1)

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 Peak Number 4 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	2.71 ng	23399	Perylene-d12	15.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentacosane	352 C25H52	000629-99-2	86
2	Tridecane, 6-propyl-	226 C16H34	055045-10-8	72
3	Sulfurous acid, butyl nonyl ester	264 C13H28O3S	1000309-17-6	64
4	Heneicosane	296 C21H44	000629-94-7	64
5	Heptacosane	380 C27H56	000593-49-7	59



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ALS Vial : 9 Sample Multiplier: 1

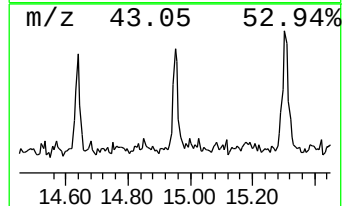
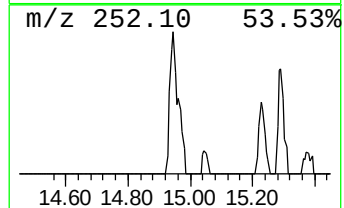
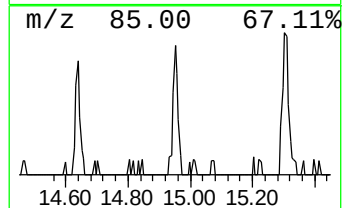
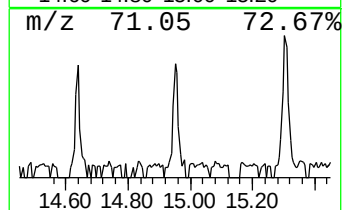
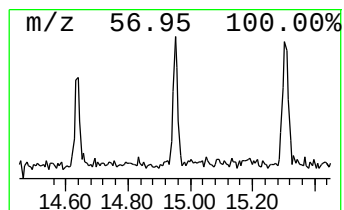
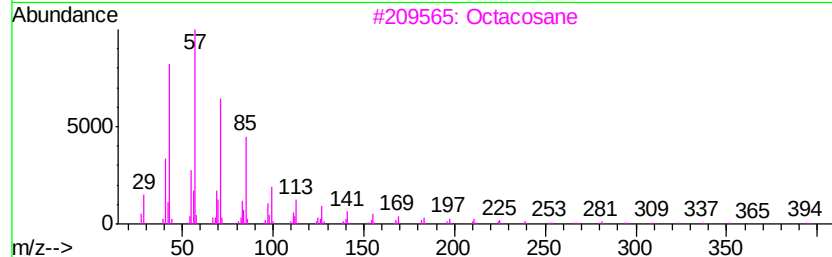
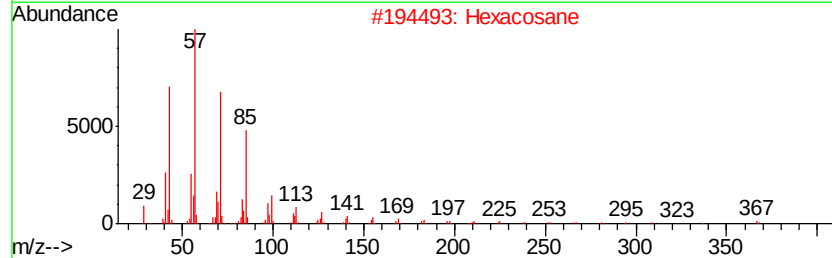
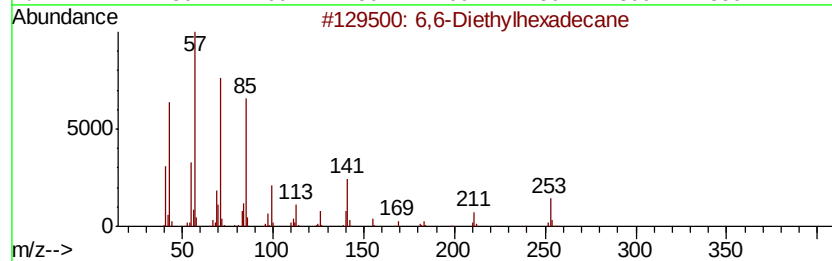
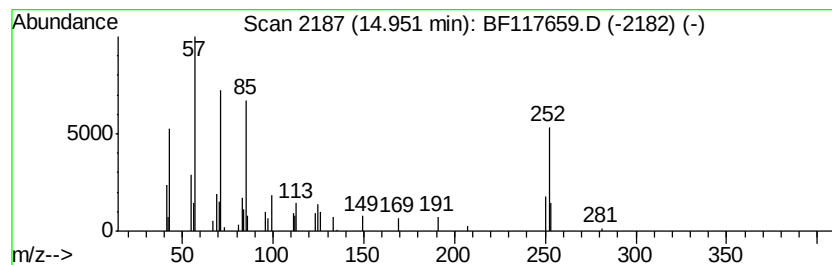
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 unknown14.95 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.		
14.95	4.55 ng	39216	Perylene-d12		15.34		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,6-Diethylhexadecane			282	C20H42	1000360-41-4	49
2	Hexacosane			366	C26H54	000630-01-3	43
3	Octacosane			394	C28H58	000630-02-4	38
4	Heptadecane			240	C17H36	000629-78-7	38
5	Hexadecane			226	C16H34	000544-76-3	38



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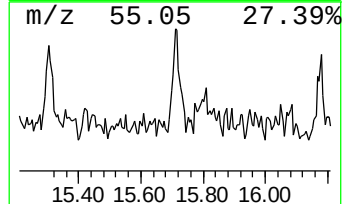
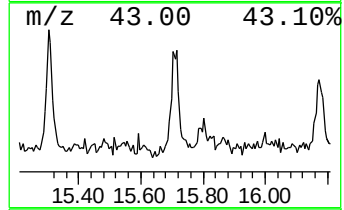
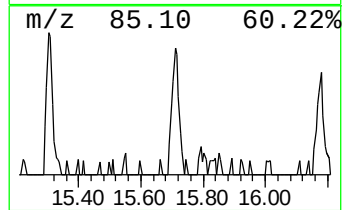
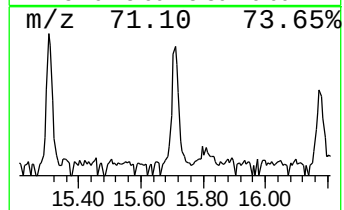
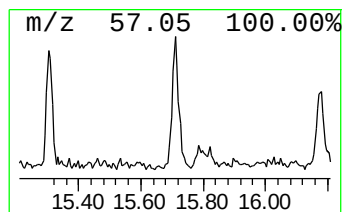
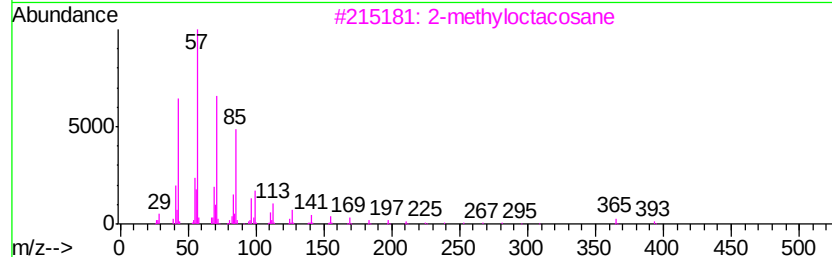
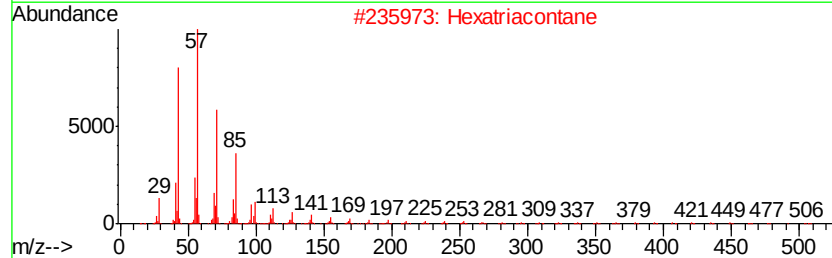
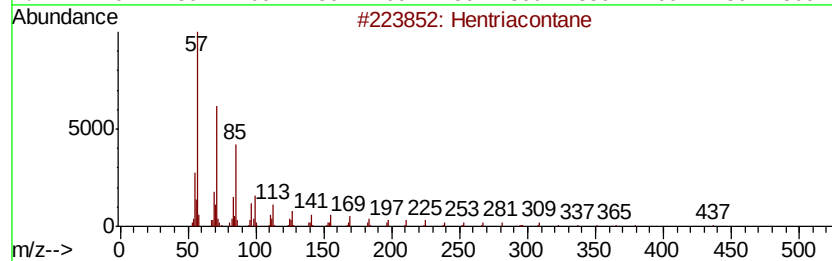
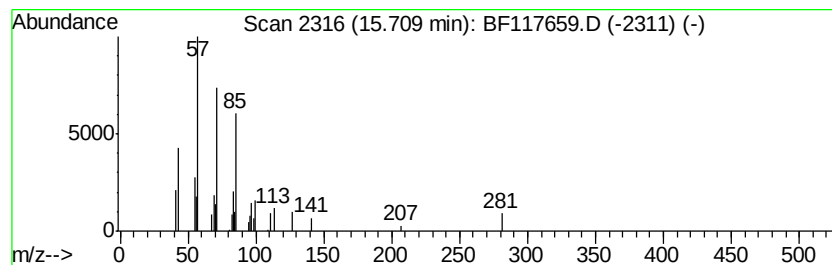
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hentriacontane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	5.16 ng	44491	Perylene-d12	15.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	91
2	Hexatriacontane		507	C36H74	000630-06-8	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Tritetracontane		605	C43H88	007098-21-7	90
5	Tetratetracontane		619	C44H90	007098-22-8	90



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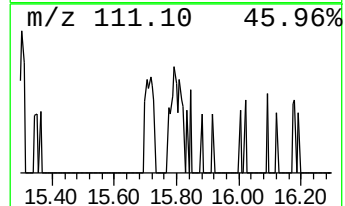
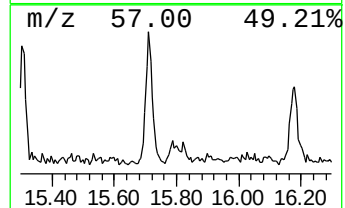
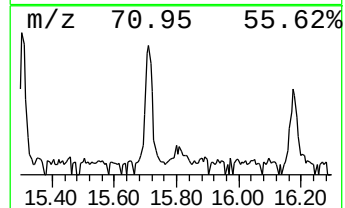
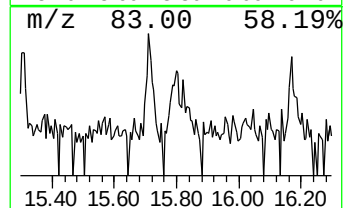
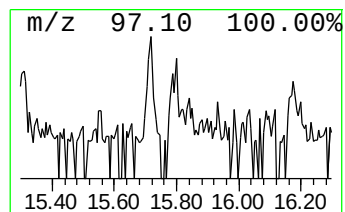
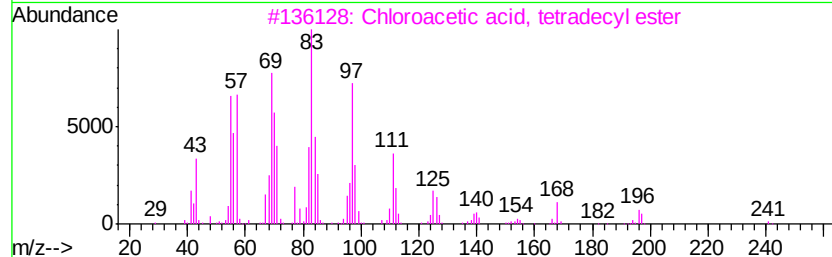
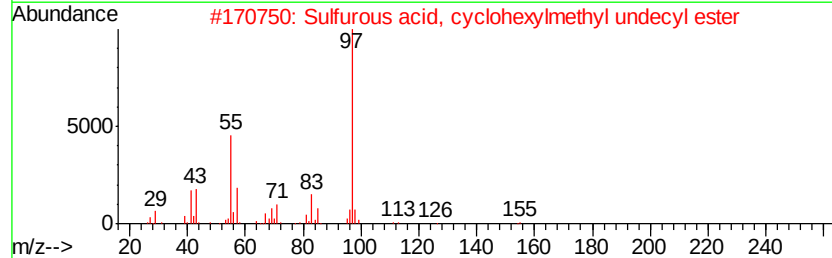
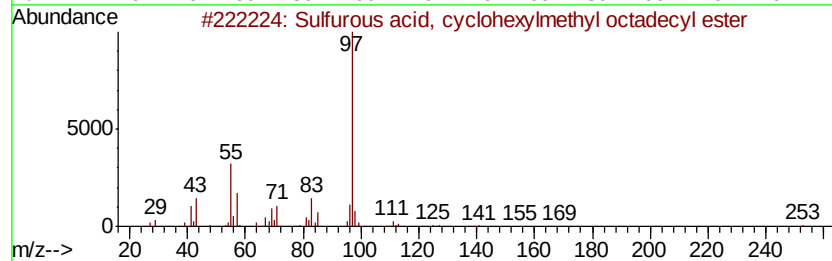
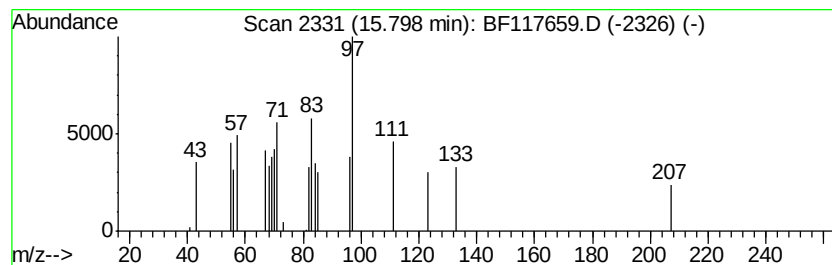
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown15.80 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	2.18 ng	18804	Perylene-d12	15.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	43
2		Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	43
3		Chloroacetic acid, tetradecyl ester	290	C16H31ClO2	018277-86-6	40
4		n-Nonadecanol-1	284	C19H40O	001454-84-8	38
5		Carbonic acid, tetradecyl 2,2,2-...	388	C17H31Cl3O3	1000314-56-0	37



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117659.D
Acq On : 31 Oct 2019 15:44
Operator : JU
Sample : K5540-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
159-46-(0-1)

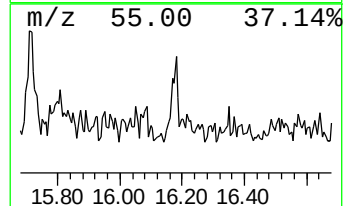
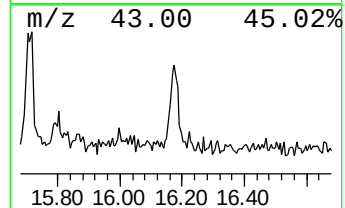
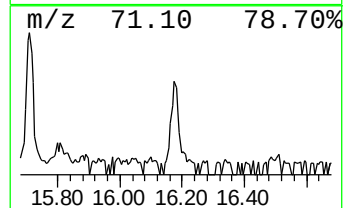
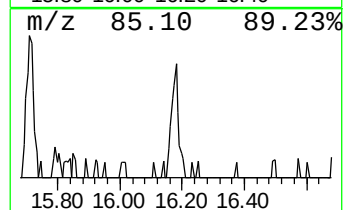
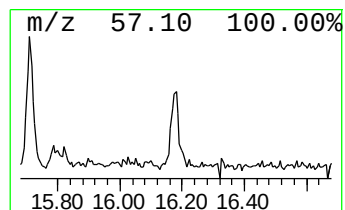
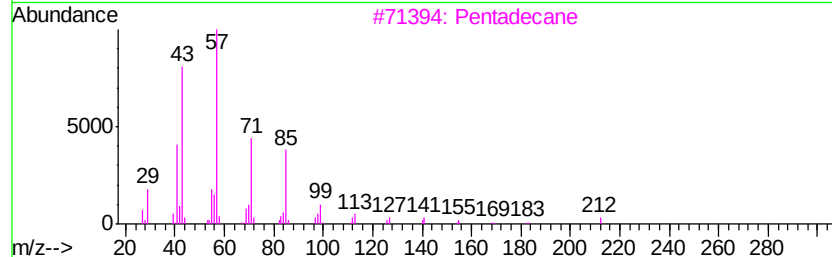
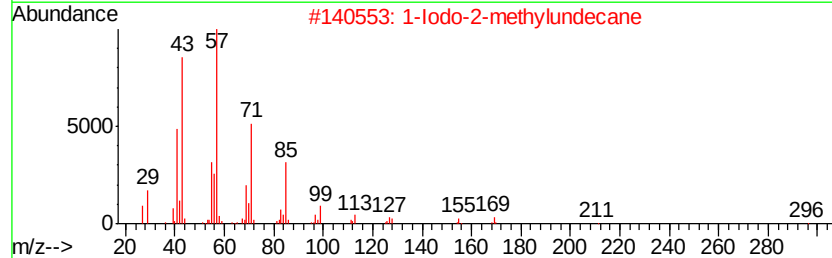
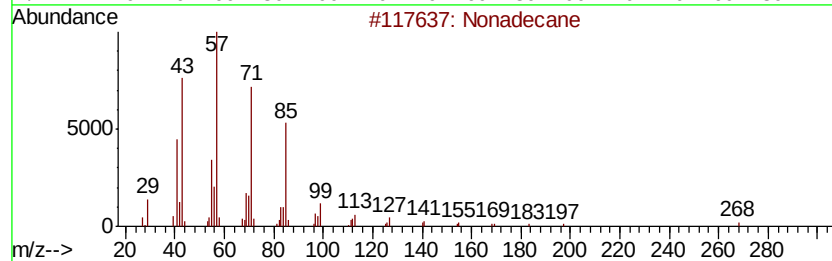
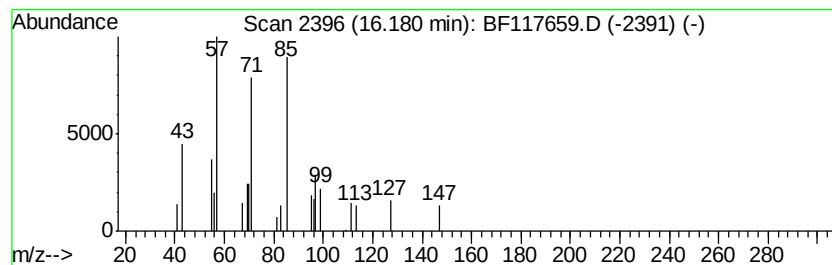
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	3.27 ng	28189	Perylene-d12	15.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	64
2	1-Iodo-2-methylundecane		296	C12H25I	073105-67-6	64
3	Pentadecane		212	C15H32	000629-62-9	59
4	Oxalic acid, 6-ethyloct-3-yl hep...		328	C19H36O4	1000309-34-5	59
5	Tritetracontane		605	C43H88	007098-21-7	56



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117659.D
Acq On : 31 Oct 2019 15:44
Operator : JU
Sample : K5540-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
159-46-(0-1)

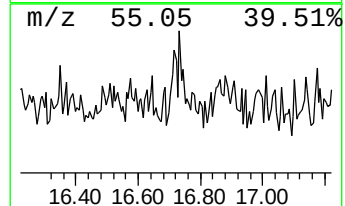
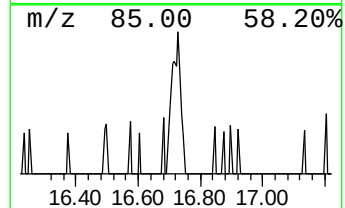
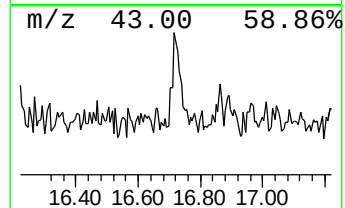
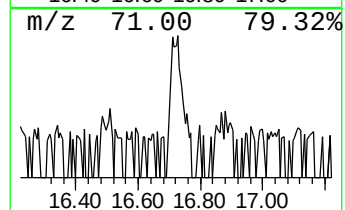
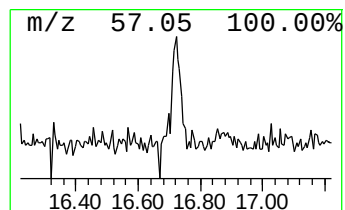
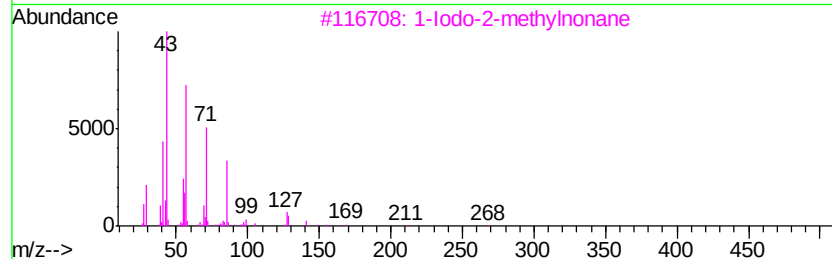
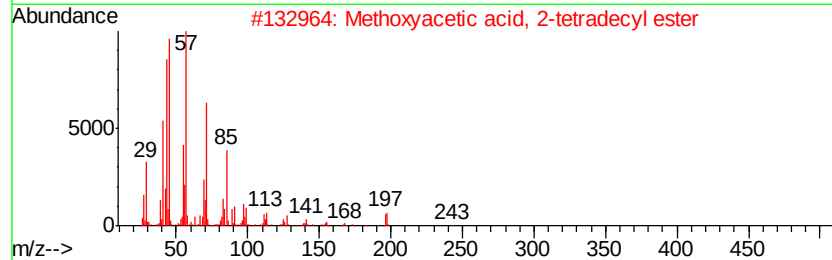
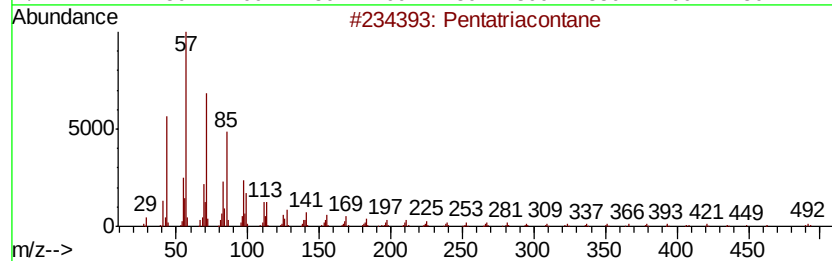
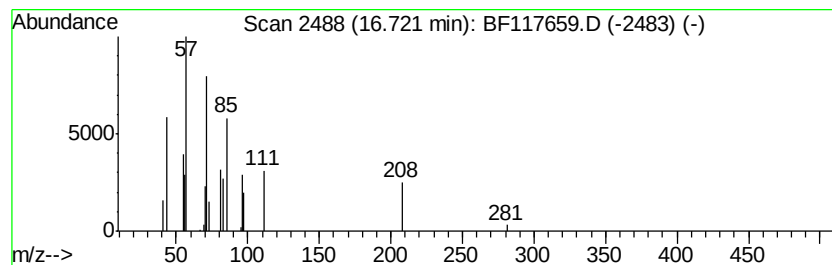
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentatriacontane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.44 ng	21008	Perylene-d12	15.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentatriacontane	493	C35H72	000630-07-9	53
2		Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	45
3		1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	43
4		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	42
5		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	42



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103119\
Data File : BF117659.D
Acq On : 31 Oct 2019 15:44
Operator : JU
Sample : K5540-17
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
159-46-(0-1)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.50	6.50	90.2	ng	793356	1	6.73	175893	20.0
Behenic alcohol	13.73	10.6	ng	112293	5	13.90	211714	20.0
Pentacosane	14.64	2.7	ng	23399	6	15.34	172436	20.0
unknown14.95	14.95	4.5	ng	39216	6	15.34	172436	20.0
Hentriacontane	15.71	5.2	ng	44491	6	15.34	172436	20.0
unknown15.80	15.80	2.2	ng	18804	6	15.34	172436	20.0
Nonadecane	16.18	3.3	ng	28189	6	15.34	172436	20.0
Pentatriacontane	16.72	2.4	ng	21008	6	15.34	172436	20.0