

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103119\
 Data File : BF117653.D
 Acq On : 31 Oct 2019 13:04
 Operator : JU
 Sample : K5540-05
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 155-98-(0-1.1)

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	582	rBV	289941	533053	78.94%	7.446%
2	6.387	728	731	747	rBV	407621	660274	97.78%	9.223%
3	6.504	747	751	761	rVV	634456	675262	100.00%	9.432%
4	6.575	761	763	776	rVB	53363	81618	12.09%	1.140%
5	6.728	786	789	797	rVB	190703	188789	27.96%	2.637%
6	6.881	812	815	825	rBV	495638	436399	64.63%	6.096%
7	7.292	882	885	906	rBV	257043	410754	60.83%	5.737%
8	8.010	1004	1007	1019	rBV	170973	231130	34.23%	3.228%
9	9.081	1186	1189	1205	rBV	560678	576456	85.37%	8.052%
10	9.486	1254	1258	1272	rBB	64417	75189	11.13%	1.050%
11	9.763	1301	1305	1322	rBB	262957	291971	43.24%	4.078%
12	10.557	1437	1440	1456	rBV	320631	397690	58.89%	5.555%
13	11.251	1555	1558	1568	rBV	249128	285766	42.32%	3.992%
14	11.775	1644	1647	1657	rBV	58995	77549	11.48%	1.083%
15	12.563	1776	1781	1786	rBV	15182	21585	3.20%	0.301%
16	12.698	1801	1804	1810	rVB2	6348	7616	1.13%	0.106%
17	12.827	1823	1826	1834	rBV	581968	563805	83.49%	7.875%
18	12.886	1834	1836	1844	rVB6	4299	10816	1.60%	0.151%
19	13.051	1859	1864	1870	rBV	12575	16438	2.43%	0.230%
20	13.392	1918	1922	1925	rBV4	18081	19289	2.86%	0.269%
21	13.727	1966	1979	1989	rBV4	71929	165083	24.45%	2.306%
22	13.898	2005	2008	2017	rBV	213341	252880	37.45%	3.532%
23	14.039	2026	2032	2036	rBV	35420	37998	5.63%	0.531%
24	14.339	2075	2083	2087	rBV	83769	99828	14.78%	1.394%
25	14.639	2128	2134	2140	rBV	136707	150322	22.26%	2.100%
26	14.704	2142	2145	2153	rBV3	21259	44674	6.62%	0.624%
27	14.845	2164	2169	2172	rBV5	4333	8897	1.32%	0.124%
28	14.951	2182	2187	2193	rBV	153187	178592	26.45%	2.495%
29	15.151	2216	2221	2222	rBV5	6092	8021	1.19%	0.112%
30	15.198	2227	2229	2235	rVB6	5221	7221	1.07%	0.101%
31	15.304	2241	2247	2250	rBV	147884	192188	28.46%	2.684%
32	15.339	2250	2253	2264	rVB2	119673	196734	29.13%	2.748%
33	15.710	2310	2316	2321	rBV	97513	139141	20.61%	1.943%
34	15.792	2326	2330	2334	rBV7	6059	11580	1.71%	0.162%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.174	2388	2395	2405	rvB2	42855	77544	11.48%	1.083%
36	16.721	2482	2488	2494	rvB4	12898	27191	4.03%	0.380%

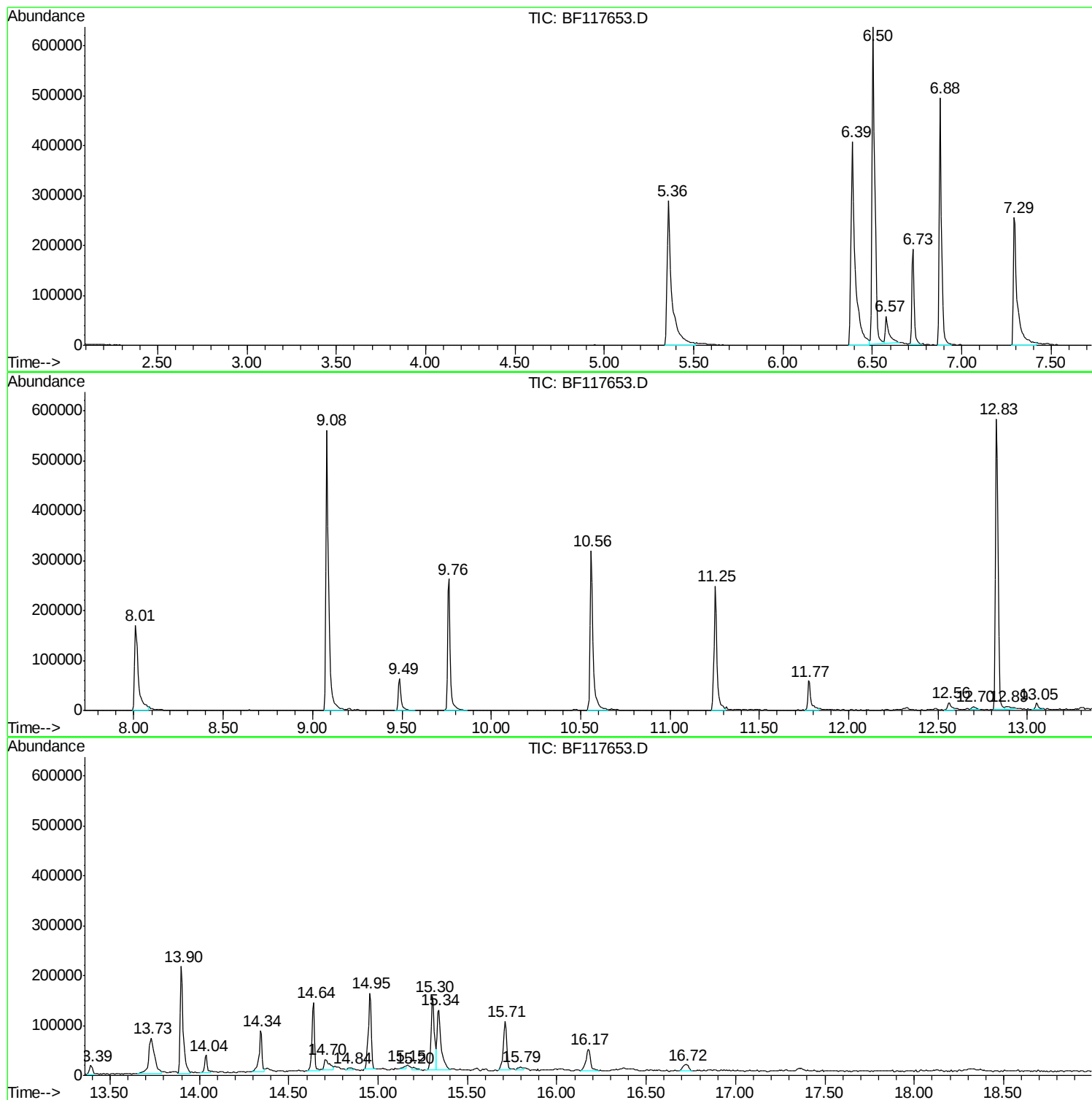
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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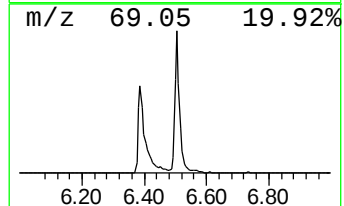
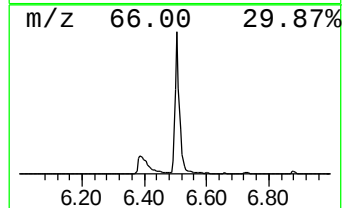
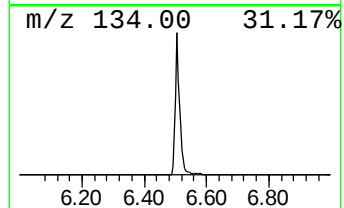
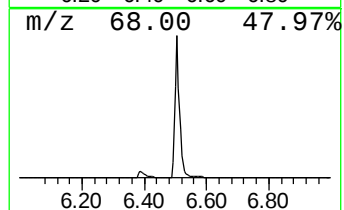
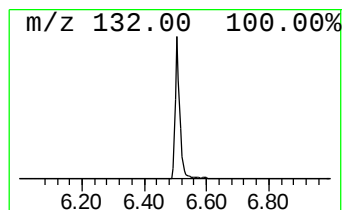
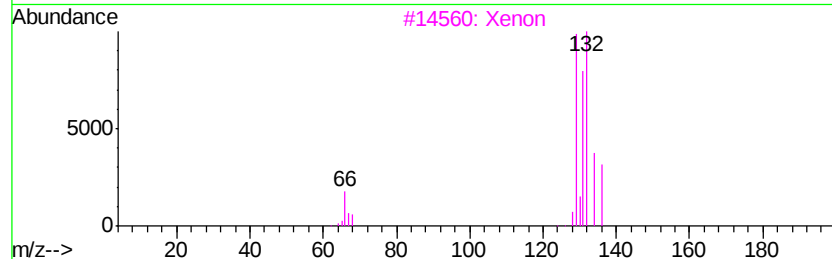
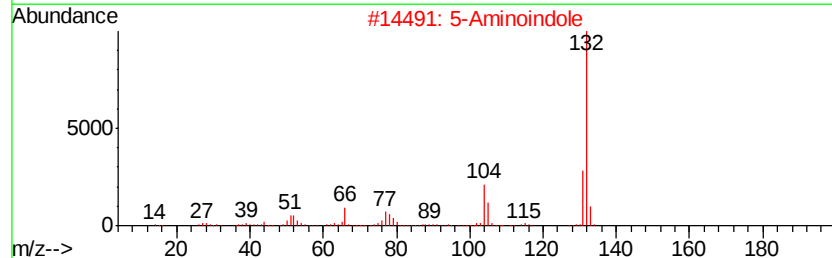
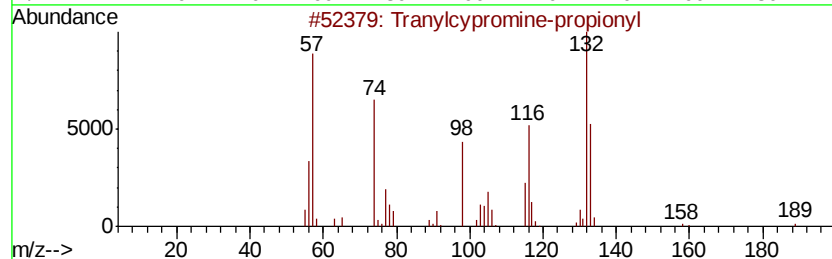
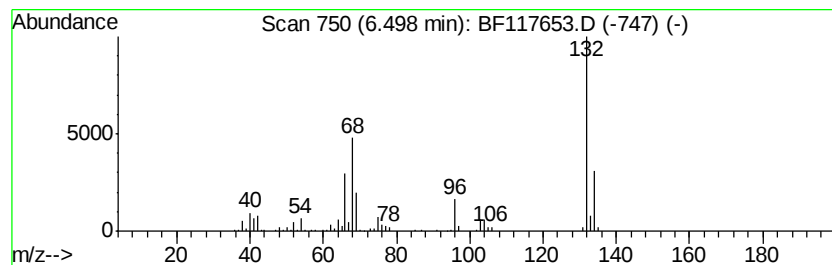
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	71.54 ng	675262	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Xenon	132	Xe	007440-63-3	9
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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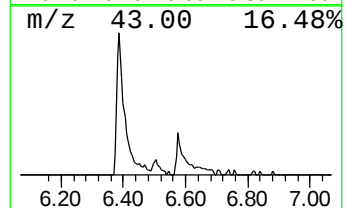
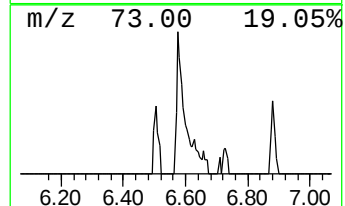
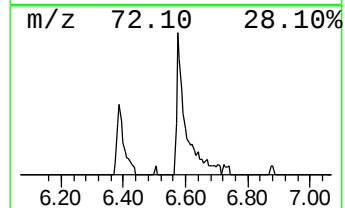
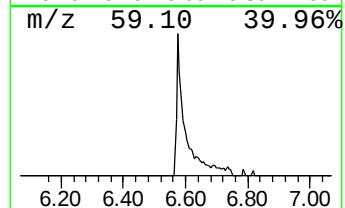
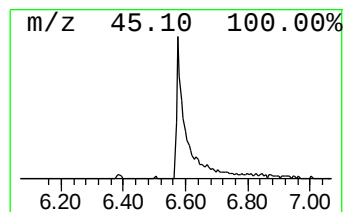
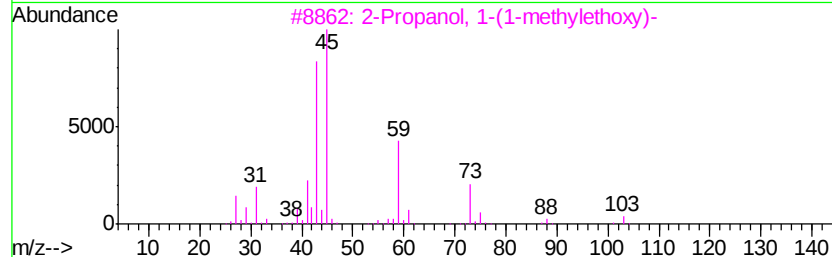
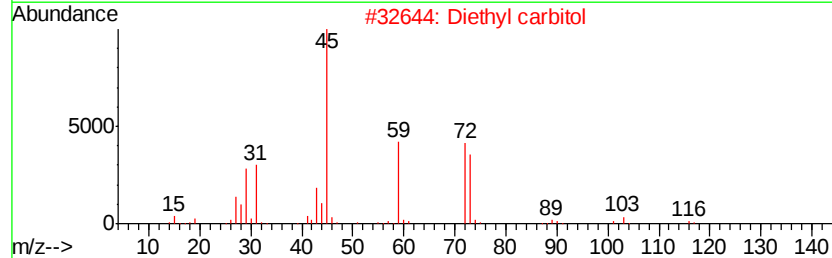
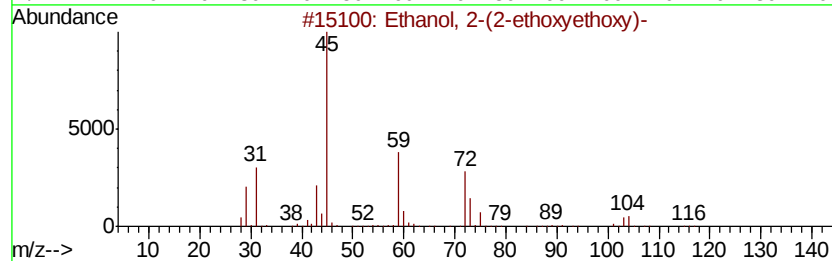
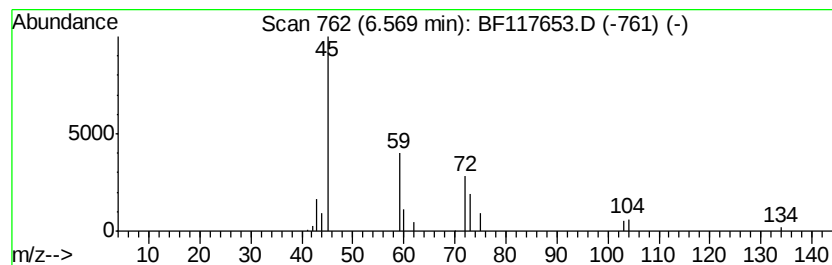
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	8.65 ng	81618	1,4-Dichlorobenzene-d4	6.73

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2		Diethyl carbitol	162	C8H18O3	000112-36-7	72
3		2-Propanol, 1-(1-methoxyethoxy)-	118	C6H14O2	003944-36-3	50
4		Ethanol, 2-[2-(2-ethoxyethoxy)et...]	178	C8H18O4	000112-50-5	45
5		Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45



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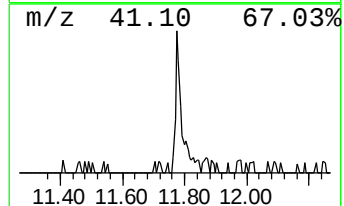
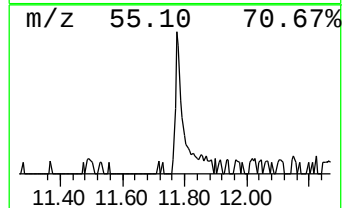
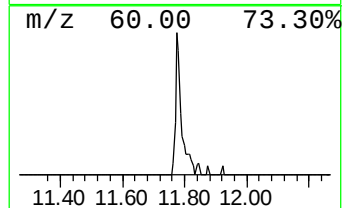
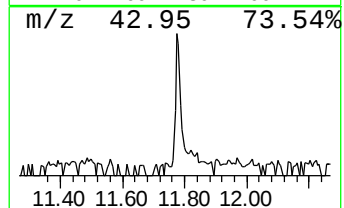
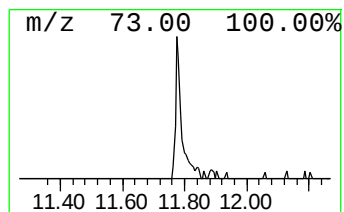
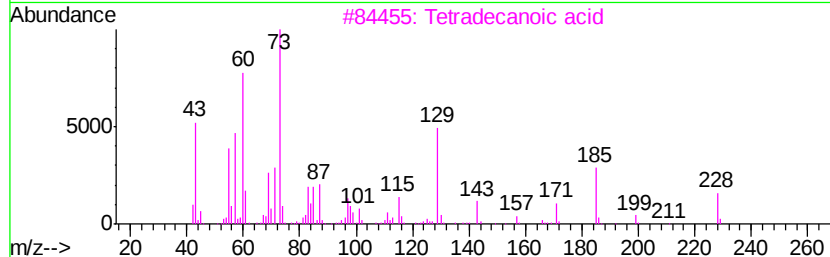
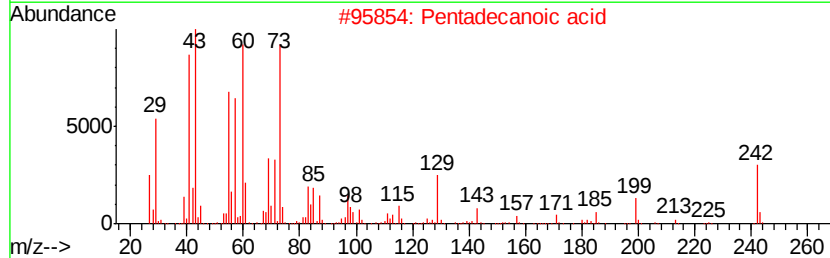
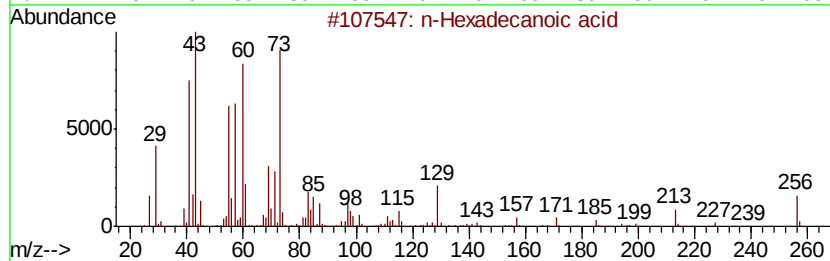
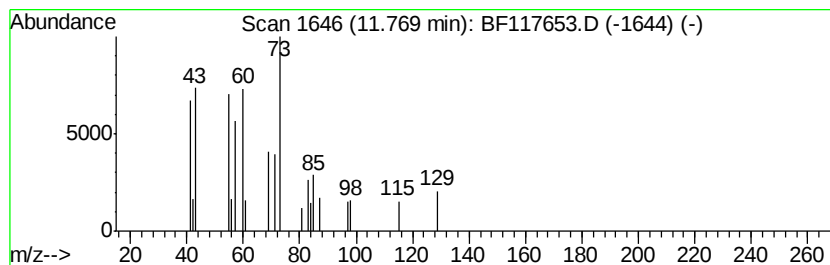
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	5.43 ng	77549	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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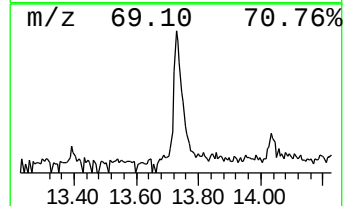
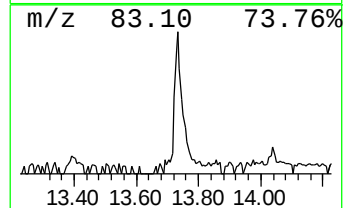
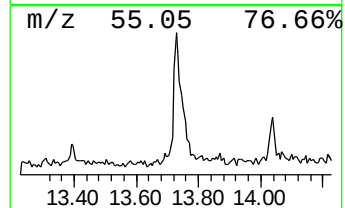
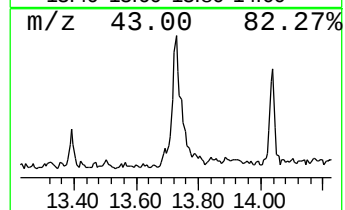
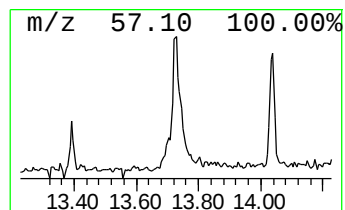
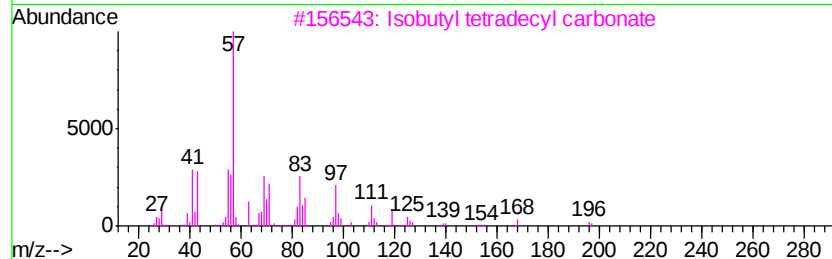
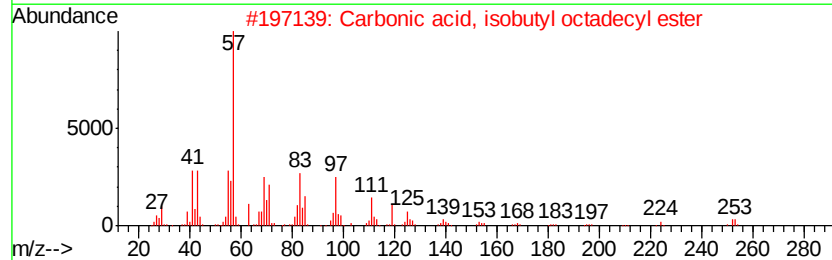
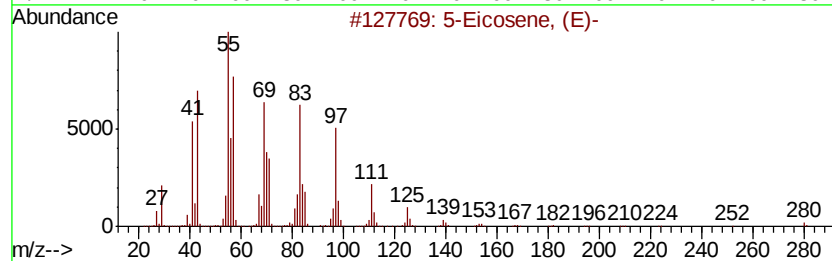
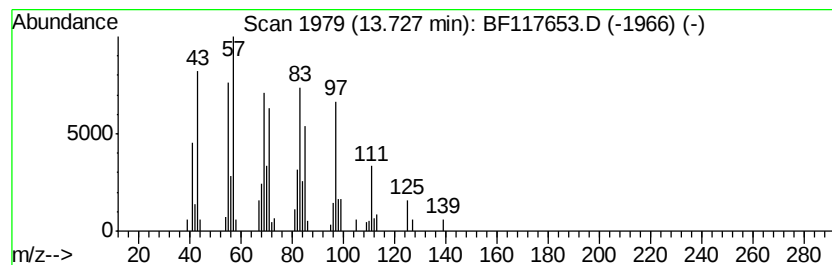
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 5-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	13.06 ng	165083	Chrysene-d12	13.90
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	5-Eicosene, (E)-	280 C20H40	074685-30-6	86
2	Carbonic acid, isobutyl octadecyl...	370 C23H46O3	1000314-61-5	86
3	Isobutyl tetradecyl carbonate	314 C19H38O3	959275-58-2	86
4	1-Hexadecanol	242 C16H34O	036653-82-4	70
5	11-Tricosene	322 C23H46	052078-56-5	59



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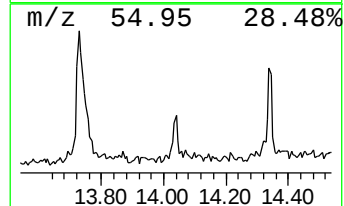
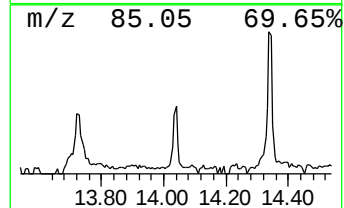
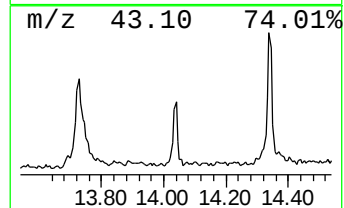
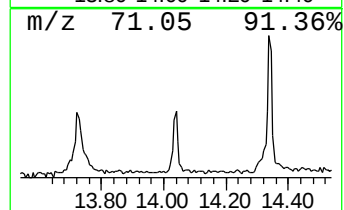
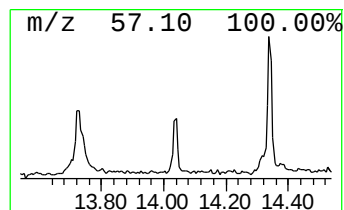
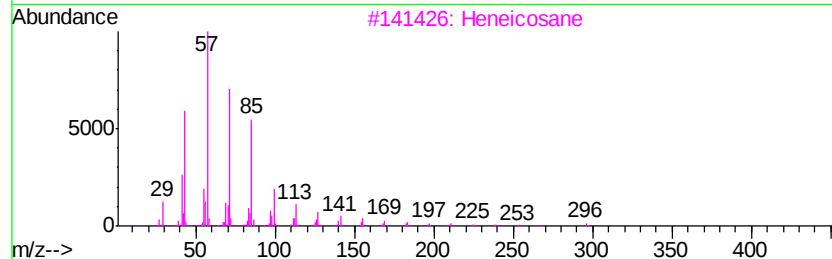
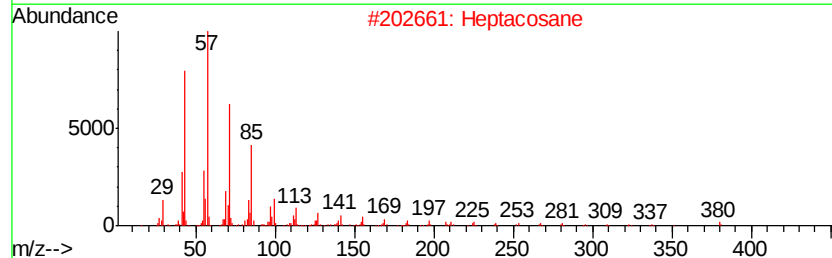
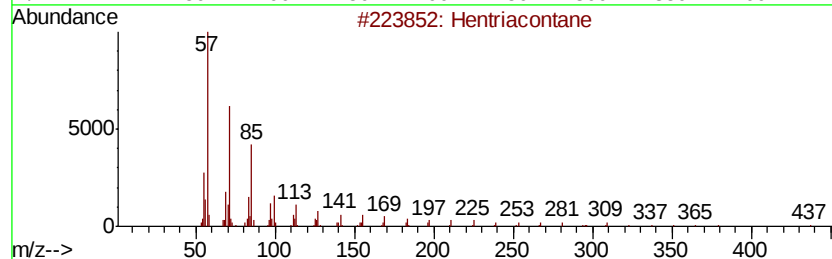
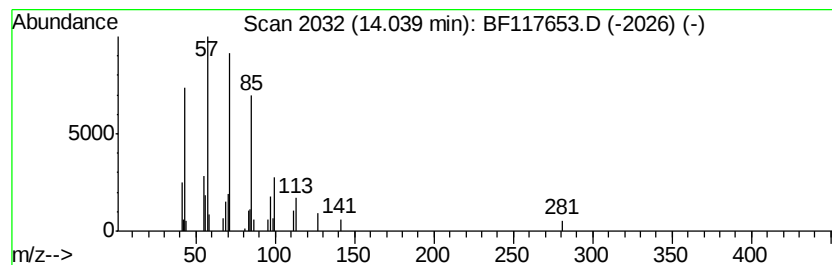
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TIC Integration Parameters: LSCINT.P

Peak Number 6 Hentriacontane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	3.01 ng	37998	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane		437	C31H64	000630-04-6	90
2	Heptacosane		380	C27H56	000593-49-7	90
3	Heneicosane		296	C21H44	000629-94-7	86
4	Heptadecane		240	C17H36	000629-78-7	86
5	Hexacosane		366	C26H54	000630-01-3	83



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117653.D
Acq On : 31 Oct 2019 13:04
Operator : JU
Sample : K5540-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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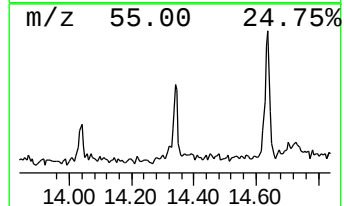
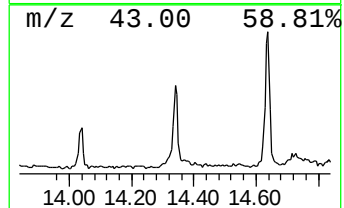
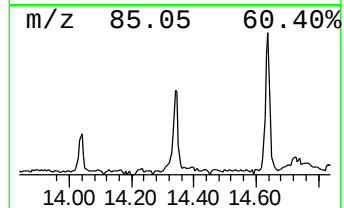
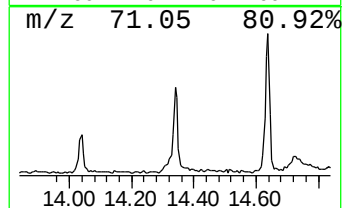
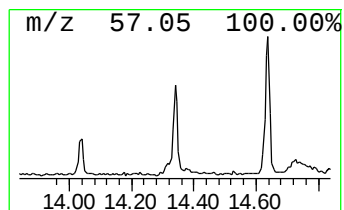
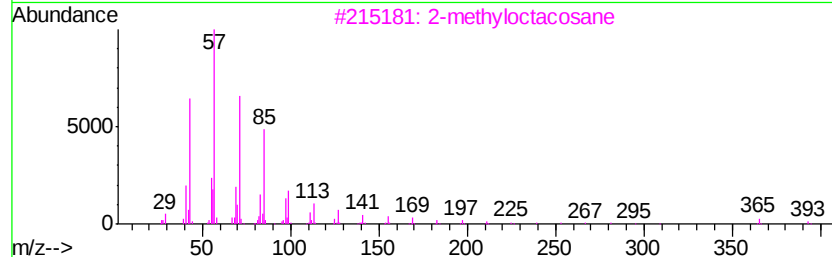
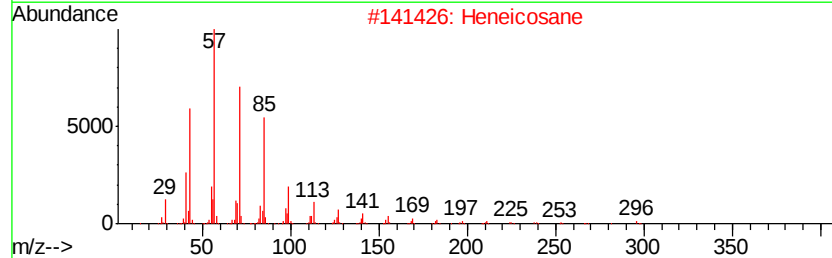
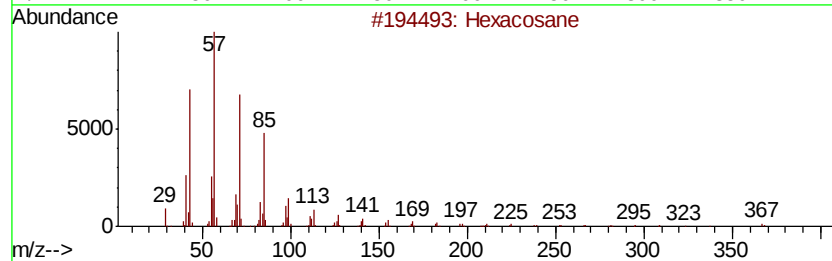
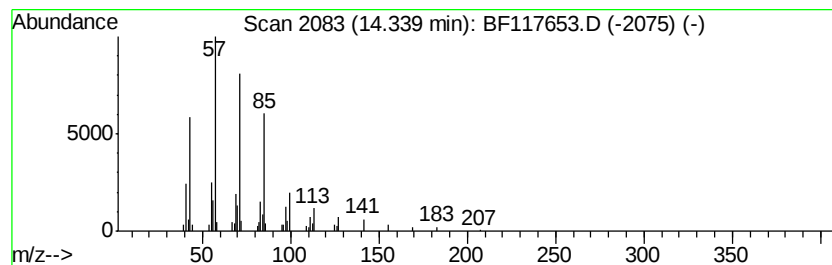
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	7.90 ng	99828	Chrysene-d12	13.90

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	91
2	Heneicosane		296	C21H44	000629-94-7	91
3	2-methyloctacosane		408	C29H60	1000376-72-8	91
4	Hentriacontane		437	C31H64	000630-04-6	91
5	Heptacosane		380	C27H56	000593-49-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117653.D
Acq On : 31 Oct 2019 13:04
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Sample : K5540-05
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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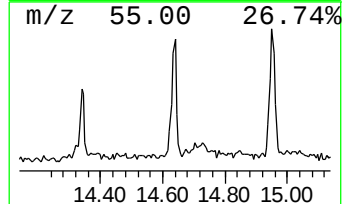
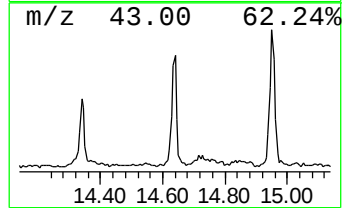
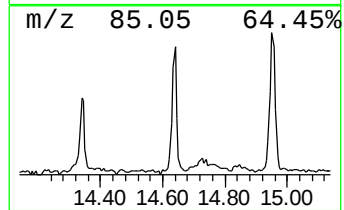
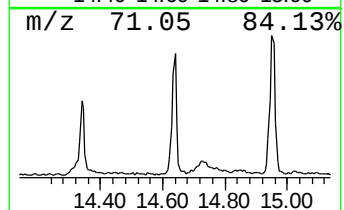
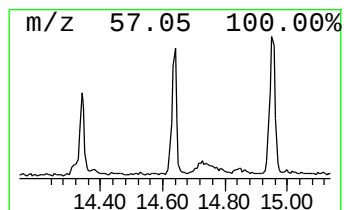
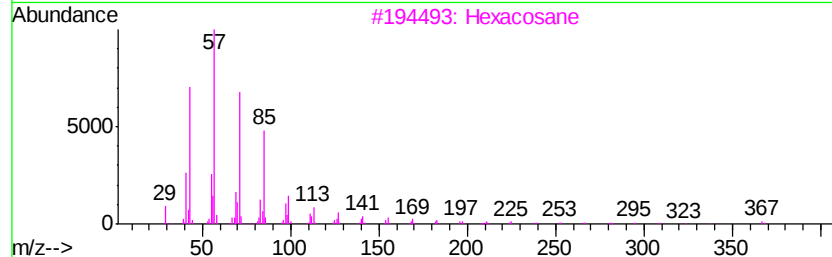
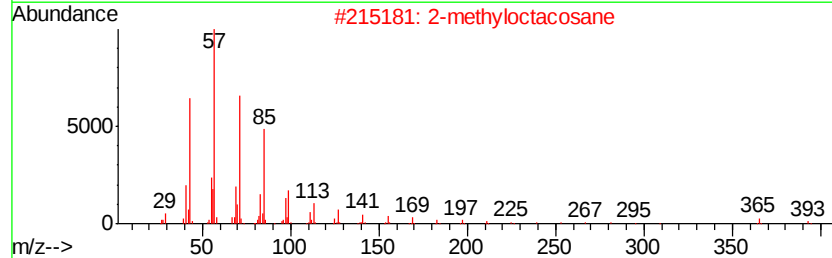
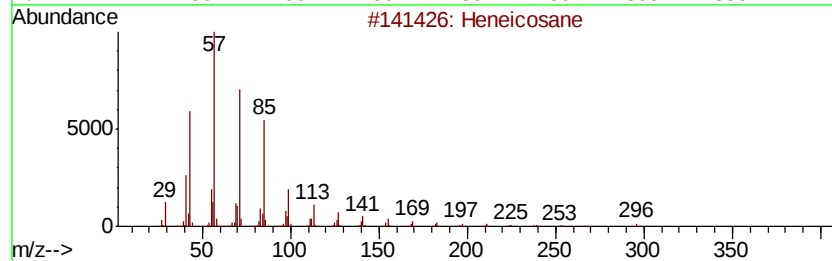
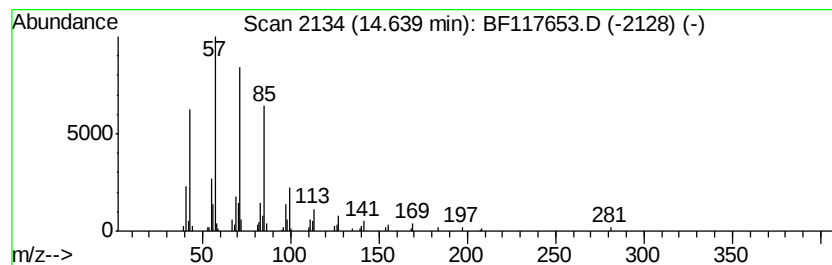
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	15.28 ng	150322	Perylene-d12	15.34

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	Heptadecane		240	C17H36	000629-78-7	90
5	Heptacosane		380	C27H56	000593-49-7	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
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Acq On : 31 Oct 2019 13:04
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Sample : K5540-05
Misc :
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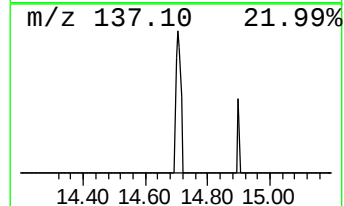
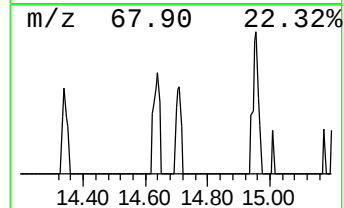
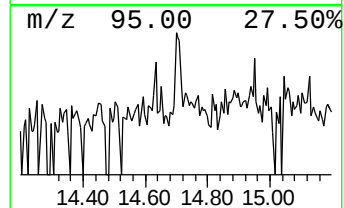
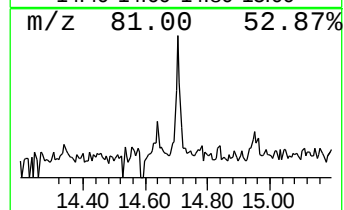
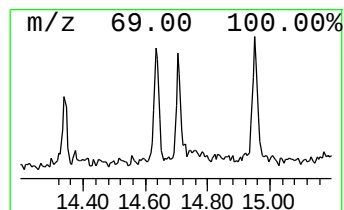
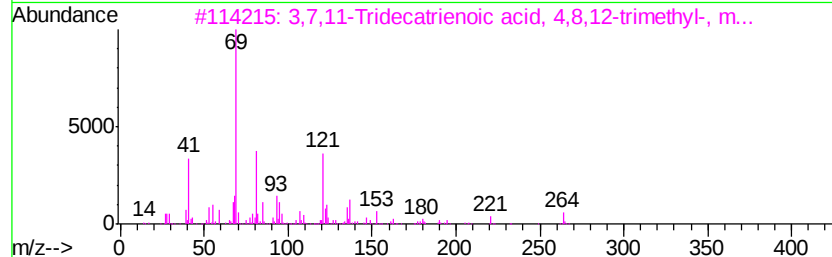
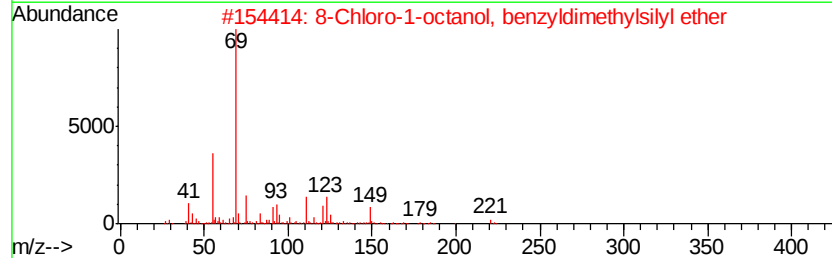
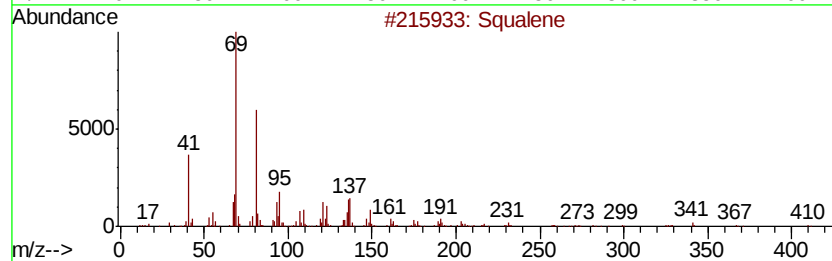
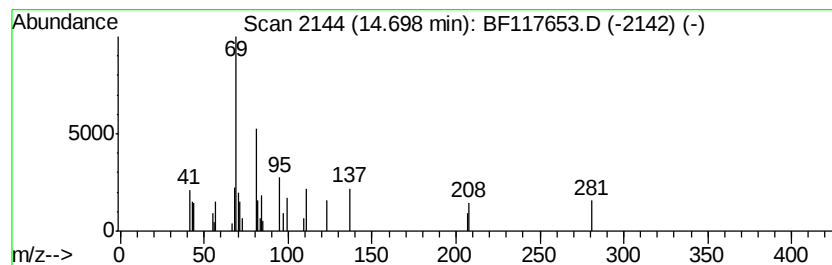
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.70	4.54 ng	44674	Perylene-d12	15.34
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	000111-02-4 72
2	8-Chloro-1-octanol, benzyldimeth...		312 C17H29ClOSi	1000375-56-9 59
3	3,7,11-Tridecatricenoic acid, 4,8...		264 C17H28O2	036237-69-1 50
4	Supraene		410 C30H50	007683-64-9 50
5	1-Hexadecyn-3-ol, 3,7,11,15-tetr...		294 C20H38O	029171-23-1 45



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117653.D
Acq On : 31 Oct 2019 13:04
Operator : JU
Sample : K5540-05
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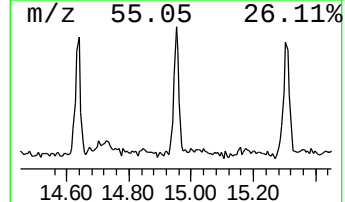
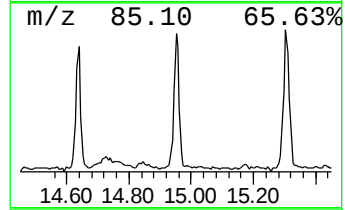
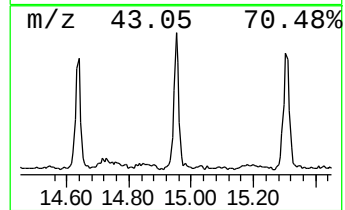
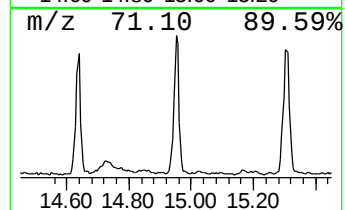
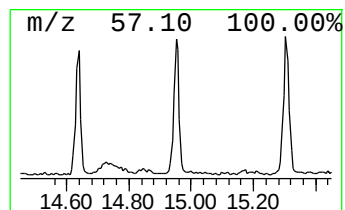
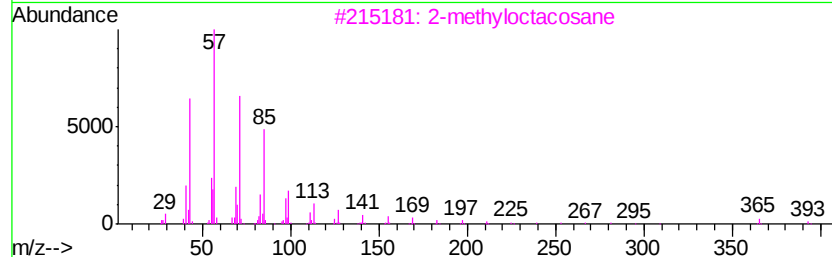
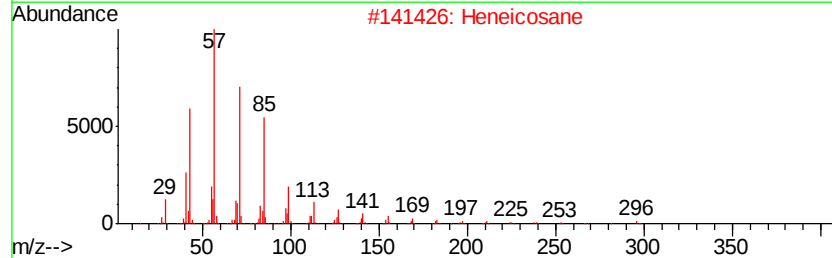
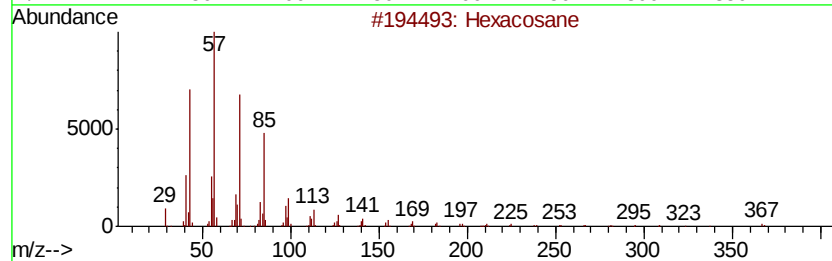
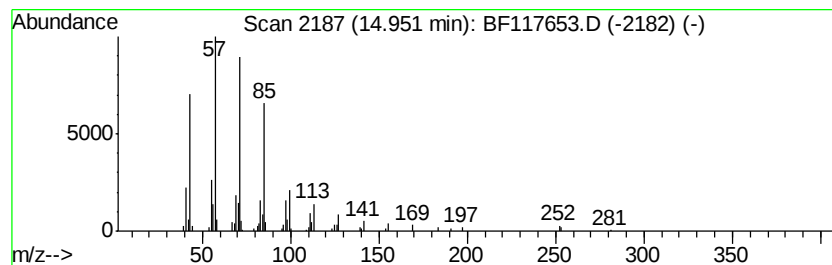
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.95	18.16 ng	178592	Perylene-d12		15.34
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heneicosane	296	C21H44	000629-94-7	91
3	2-methvloctacosane	408	C29H60	1000376-72-8	91
4	Heptadecane	240	C17H36	000629-78-7	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117653.D
Acq On : 31 Oct 2019 13:04
Operator : JU
Sample : K5540-05
Misc :
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ClientSampleId :
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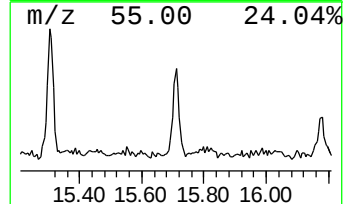
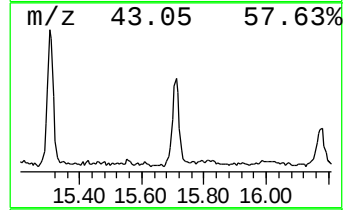
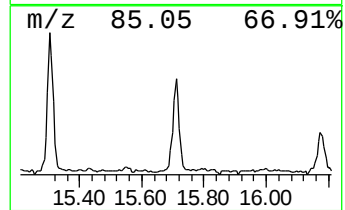
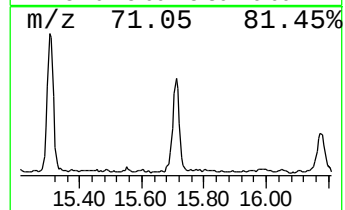
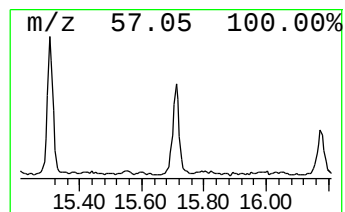
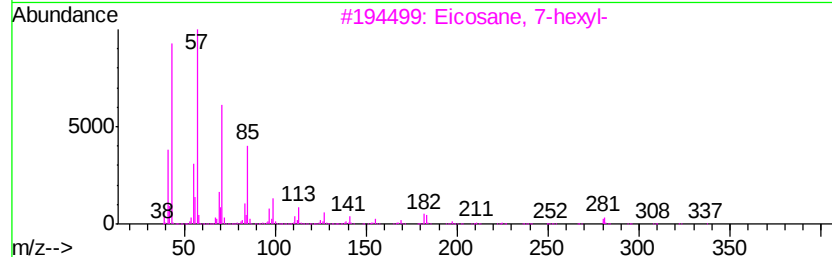
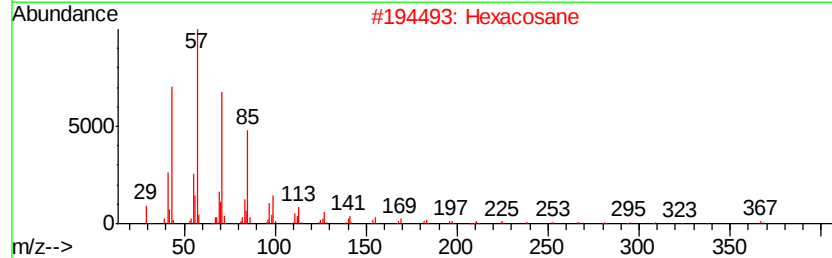
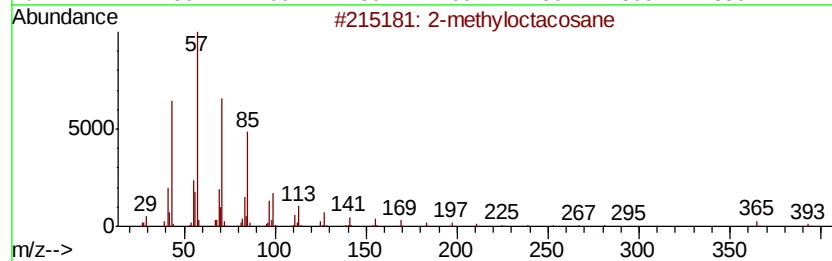
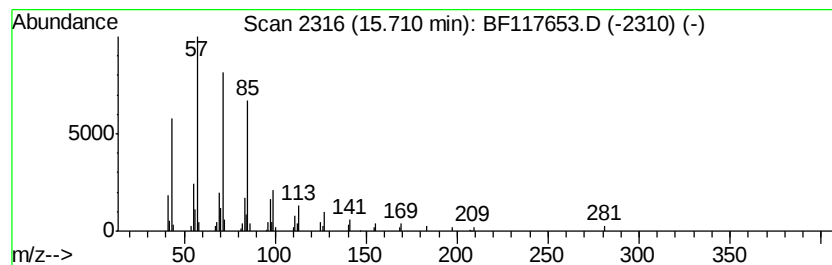
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	14.15 ng	139141	Perylene-d12	15.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Hexacosane	366	C26H54	000630-01-3	90
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4		Heneicosane	296	C21H44	000629-94-7	87
5		Heptadecane	240	C17H36	000629-78-7	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117653.D
Acq On : 31 Oct 2019 13:04
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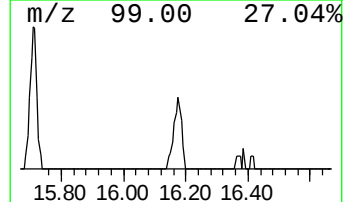
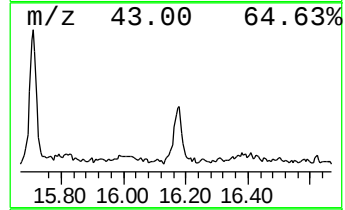
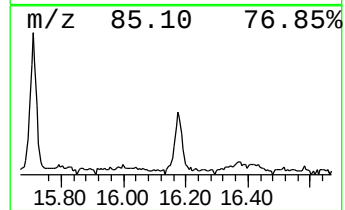
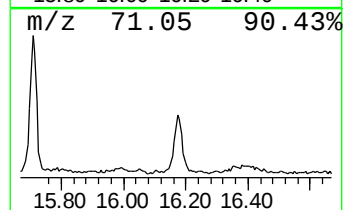
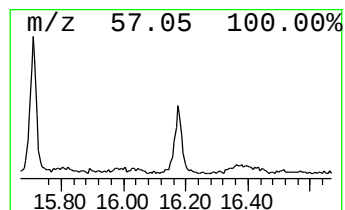
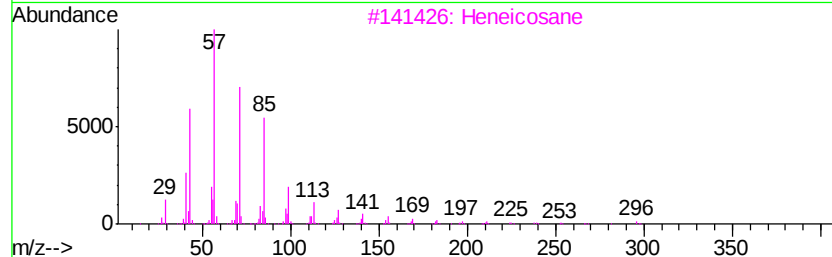
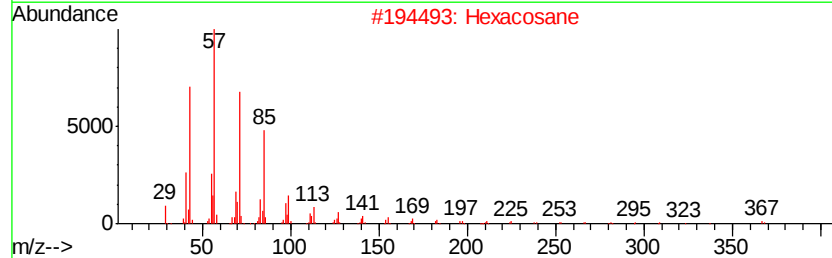
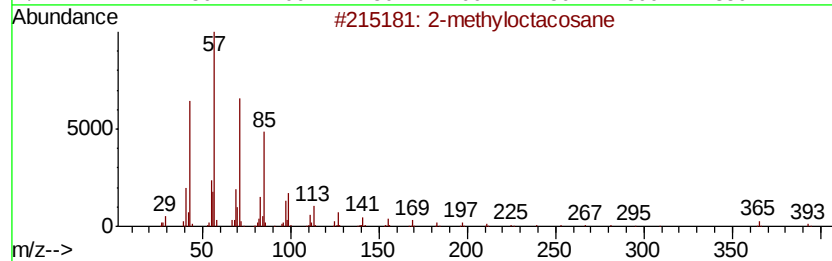
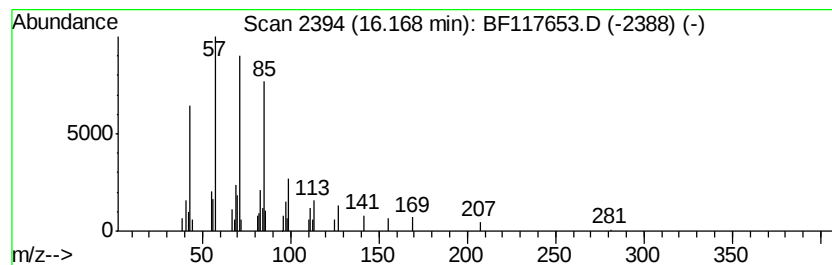
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Methoxyacetic acid, 2-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	7.88 ng	77544	Perylene-d12	15.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-methyloctacosane	408	C29H60	1000376-72-8	91
2			Hexacosane	366	C26H54	000630-01-3	90
3			Heneicosane	296	C21H44	000629-94-7	87
4			Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	86
5			2-methyltetracosane	352	C25H52	1000376-72-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103119\
Data File : BF117653.D
Acq On : 31 Oct 2019 13:04
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ALS Vial : 3 Sample Multiplier: 1

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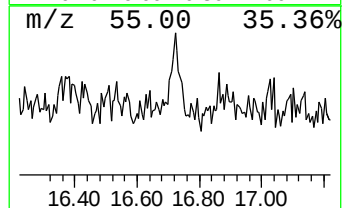
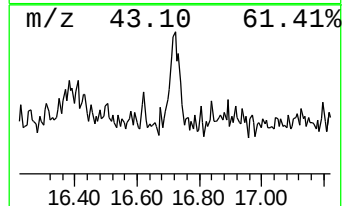
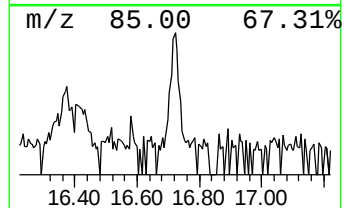
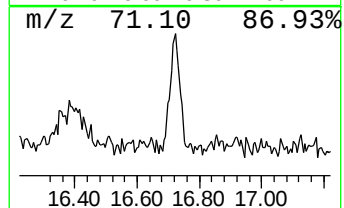
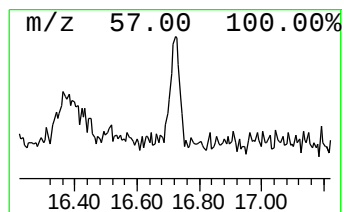
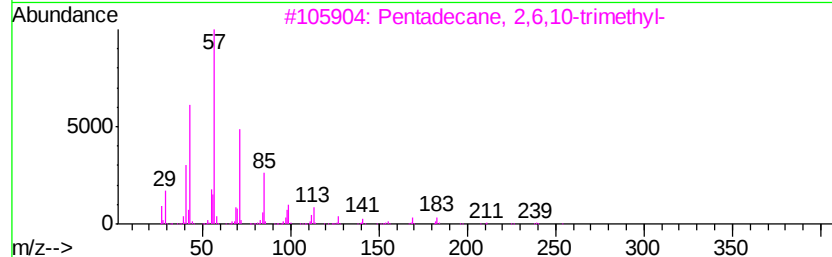
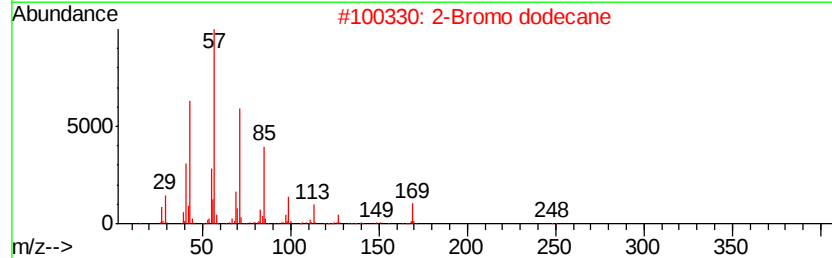
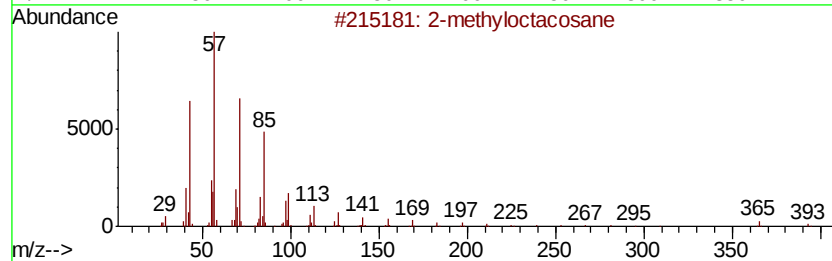
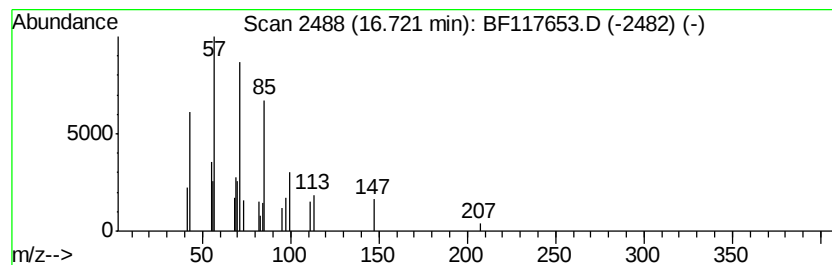
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101819.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-Bromo dodecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	2.76 ng	27191	Perylene-d12	15.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	72
2		2-Bromo dodecane	248	C12H25Br	013187-99-0	64
3		Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	64
4		Heptadecane	240	C17H36	000629-78-7	64
5		Pentacosane	352	C25H52	000629-99-2	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF103119\
 Data File : BF117653.D
 Acq On : 31 Oct 2019 13:04
 Operator : JU
 Sample : K5540-05
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 155-98-(0-1.1)

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	71.5	ng	675262	1	6.73	188789	20.0
Ethanol, 2-(2-eth...	6.57	8.7	ng	81618	1	6.73	188789	20.0
n-Hexadecanoic acid	11.77	5.4	ng	77549	4	11.25	285766	20.0
5-Eicosene, (E)-	13.73	13.1	ng	165083	5	13.90	252880	20.0
Hentriacontane	14.04	3.0	ng	37998	5	13.90	252880	20.0
Hexacosane	14.34	7.9	ng	99828	5	13.90	252880	20.0
Heneicosane	14.64	15.3	ng	150322	6	15.34	196734	20.0
Squalene	14.70	4.5	ng	44674	6	15.34	196734	20.0
Heptadecane	14.95	18.2	ng	178592	6	15.34	196734	20.0
2-methyloctacosane	15.71	14.2	ng	139141	6	15.34	196734	20.0
Methoxyacetic aci...	16.17	7.9	ng	77544	6	15.34	196734	20.0
2-Bromo dodecane	16.72	2.8	ng	27191	6	15.34	196734	20.0