

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
 Data File : BF113204.D
 Acq On : 21 Mar 2019 13:11
 Operator : JU/SJ
 Sample : K1688-33 10X
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JC-02-031919-G

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-BF022719.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	5.334	548	552	563	rBV	196476	238624	9.84%	1.355%
2	6.363	723	727	740	rBV	222805	285393	11.77%	1.621%
3	6.492	745	749	757	rVV	292527	287018	11.84%	1.630%
4	6.722	784	788	798	rBV	946043	841273	34.70%	4.778%
5	6.875	811	814	822	rBV	251812	228112	9.41%	1.295%
6	7.281	877	883	890	rBV	134720	156764	6.47%	0.890%
7	8.004	1002	1006	1013	rBV	1269075	1185808	48.91%	6.734%
8	8.604	1104	1108	1115	rBV5	35192	53596	2.21%	0.304%
9	9.075	1185	1188	1199	rBV	385770	426467	17.59%	2.422%
10	9.169	1201	1204	1208	rVB	69859	59551	2.46%	0.338%
11	9.475	1253	1256	1260	rBV2	39168	66908	2.76%	0.380%
12	9.698	1291	1294	1298	rBV	85249	73688	3.04%	0.418%
13	9.751	1298	1303	1312	rBV	1425331	1440660	59.42%	8.181%
14	9.939	1329	1335	1336	rBV4	16629	29857	1.23%	0.170%
15	10.192	1375	1378	1381	rBV	111770	84814	3.50%	0.482%
16	10.416	1409	1416	1419	rBV	48254	66477	2.74%	0.378%
17	10.539	1433	1437	1442	rBV	253171	264596	10.91%	1.503%
18	10.663	1456	1458	1466	rVB	117458	145013	5.98%	0.824%
19	11.110	1531	1534	1537	rBV	96337	89924	3.71%	0.511%
20	11.145	1537	1540	1544	rVB	41285	43527	1.80%	0.247%
21	11.233	1551	1555	1562	rBV	1546442	1388090	57.25%	7.883%
22	11.539	1604	1607	1609	rBV	96655	83271	3.43%	0.473%
23	11.633	1620	1623	1631	rVB	903971	751389	30.99%	4.267%
24	11.769	1643	1646	1654	rBV	160475	184069	7.59%	1.045%
25	11.939	1670	1675	1679	rBV	75799	85173	3.51%	0.484%
26	12.316	1735	1739	1741	rBV	2485168	2424665	100.00%	13.770%
27	12.339	1741	1743	1746	rVB	2804069	2244995	92.59%	12.749%
28	12.421	1754	1757	1761	rBV	453671	395452	16.31%	2.246%
29	12.474	1761	1766	1774	rVV5	73555	170661	7.04%	0.969%
30	12.551	1777	1779	1785	rVB4	55203	68394	2.82%	0.388%
31	12.657	1794	1797	1802	rVB3	88210	90273	3.72%	0.513%
32	12.698	1802	1804	1807	rBV	62537	54204	2.24%	0.308%
33	12.810	1820	1823	1829	rBV	395872	362228	14.94%	2.057%
34	12.980	1849	1852	1854	rBV	71235	69300	2.86%	0.394%

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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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35	13.057	1862	1865	1870	rVB3	79167	114579	4.73%	0.651%
36	13.145	1877	1880	1883	rBV	70432	54795	2.26%	0.311%
37	13.398	1920	1923	1926	rBV	52105	47575	1.96%	0.270%
38	13.721	1975	1978	1981	rBV	62825	61119	2.52%	0.347%
39	13.815	1991	1994	1998	rBV2	39183	40553	1.67%	0.230%
40	13.863	1998	2002	2009	rVV	1137749	1087076	44.83%	6.173%
41	14.039	2029	2032	2035	rBV	80574	70571	2.91%	0.401%
42	14.339	2081	2083	2087	rBV	104180	111511	4.60%	0.633%
43	14.633	2131	2133	2140	rBV	124979	134904	5.56%	0.766%
44	14.951	2184	2187	2193	rVB	139963	172681	7.12%	0.981%
45	15.274	2237	2242	2245	rBV	917413	1130993	46.65%	6.423%
46	15.709	2313	2316	2321	rVB	106478	142229	5.87%	0.808%

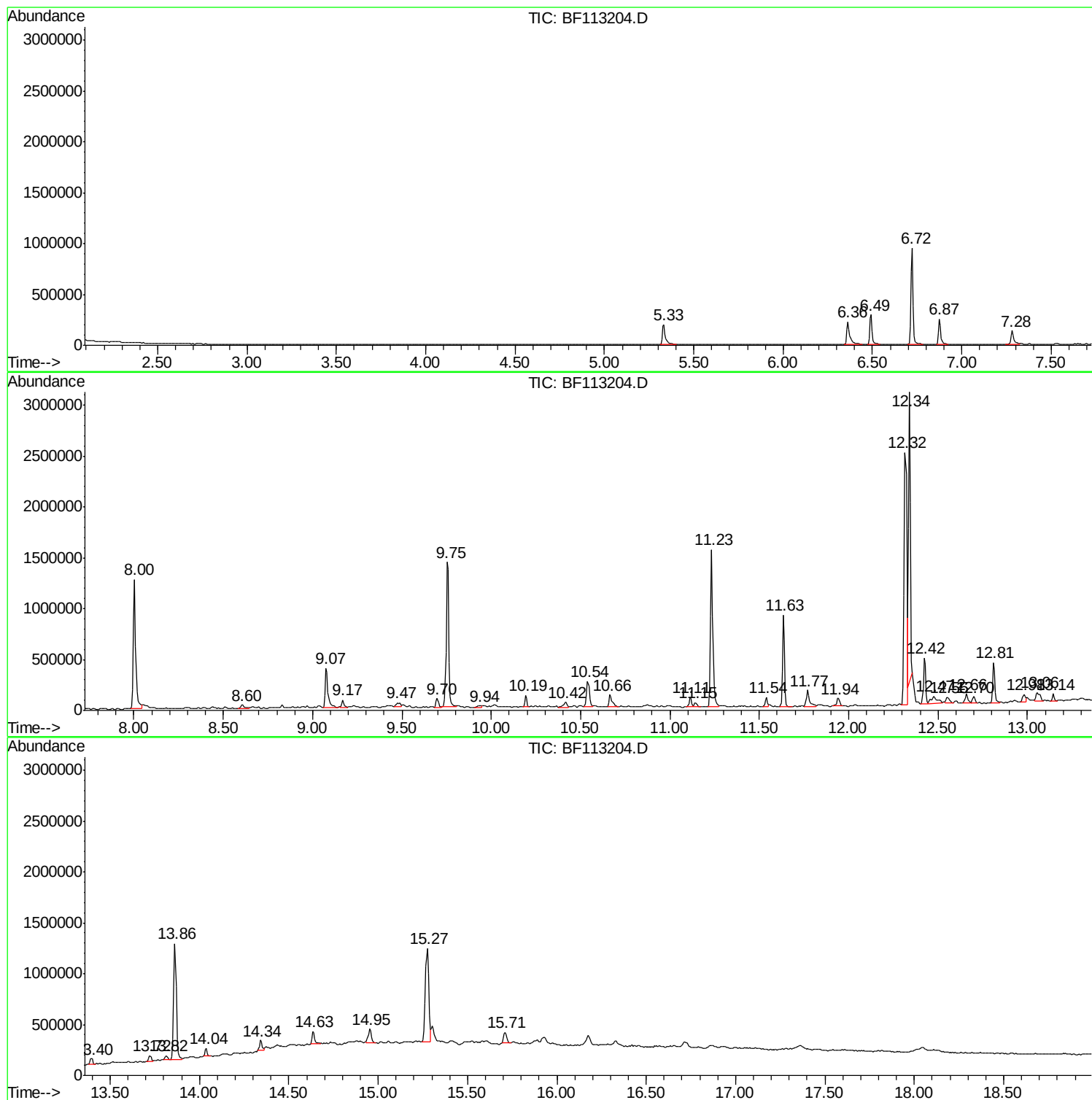
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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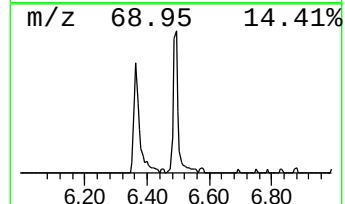
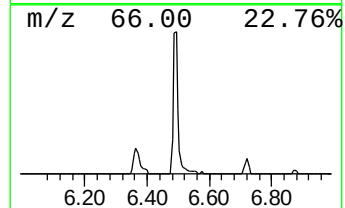
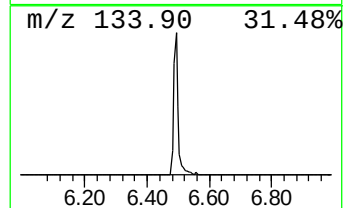
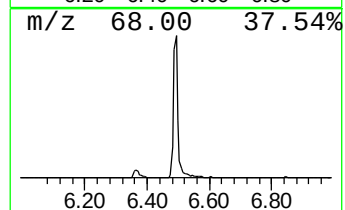
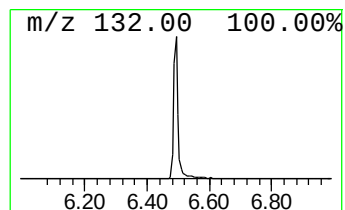
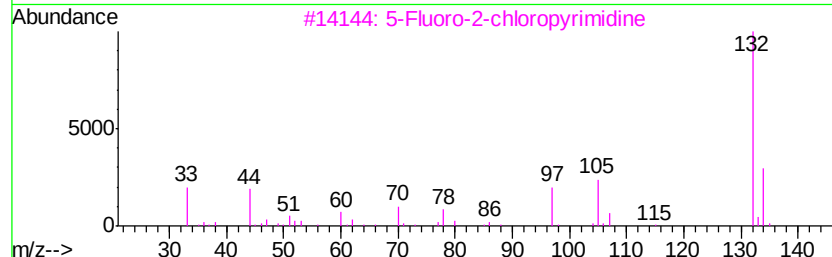
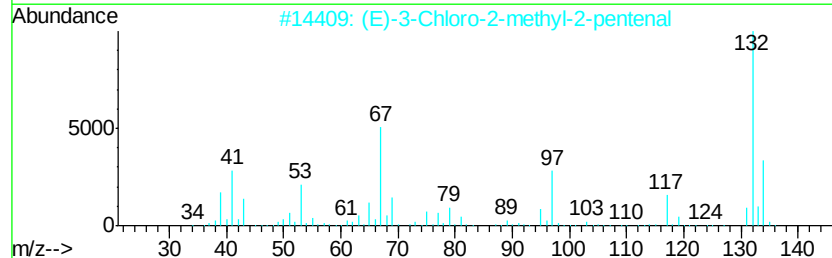
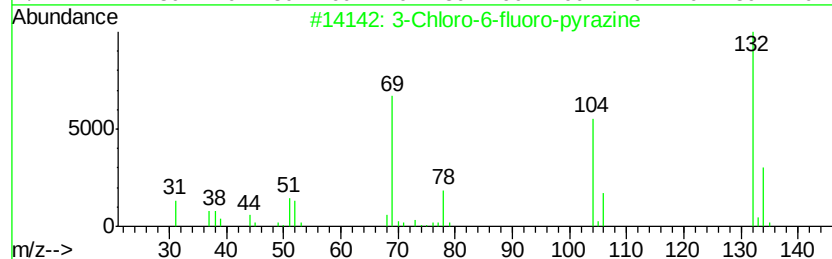
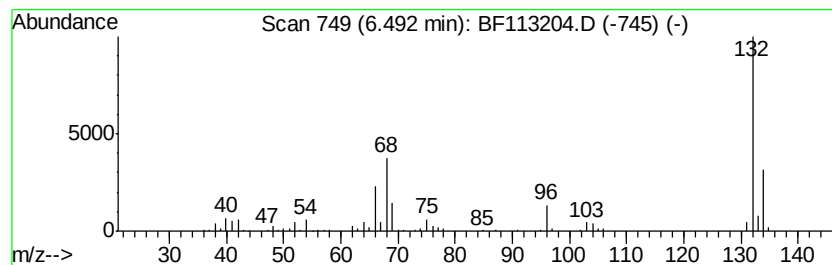
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.49 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	6.82 ng	287018	1,4-Dichlorobenzene-d4	6.72

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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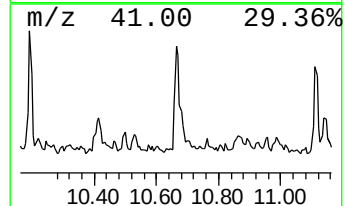
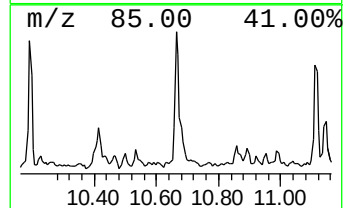
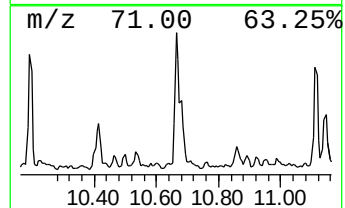
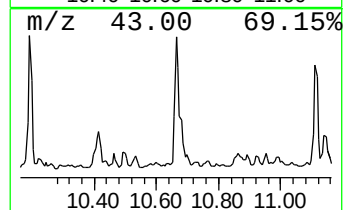
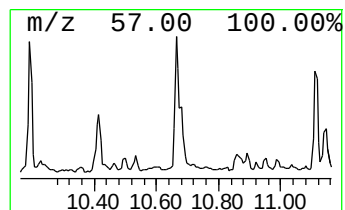
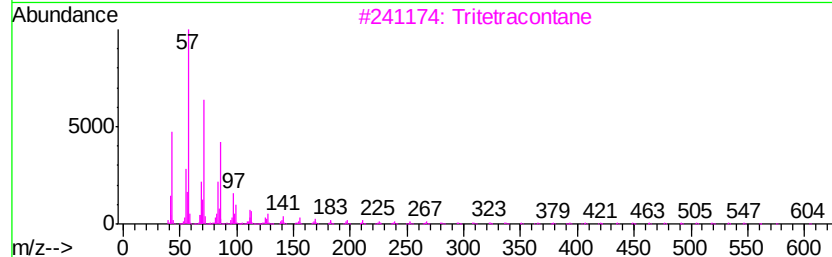
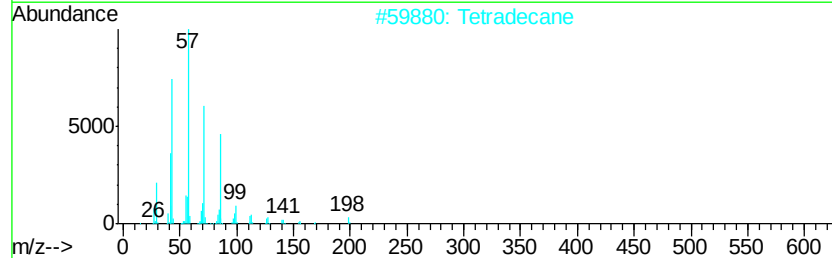
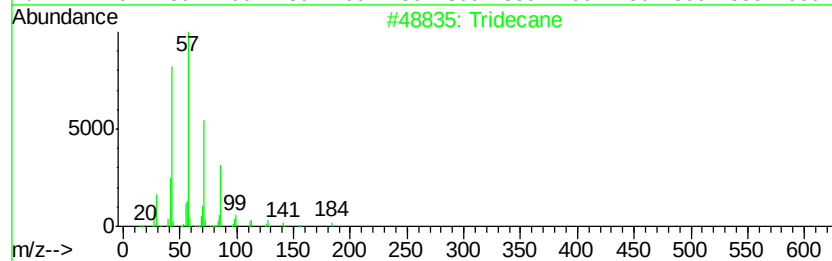
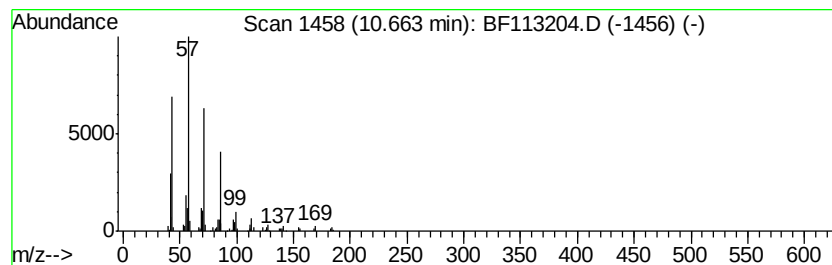
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Tridecane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD		R.T.
10.66	2.09 ng	145013	Phenanthrene-d10		11.23
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Tetradecane	198	C14H30	000629-59-4	91
3	Tritetracontane	605	C43H88	007098-21-7	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87



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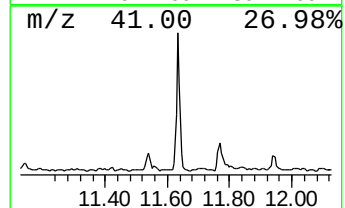
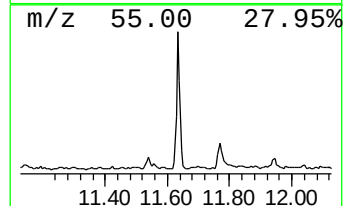
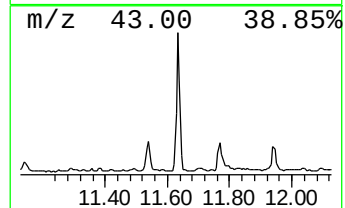
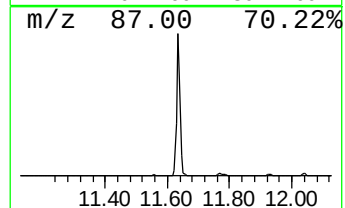
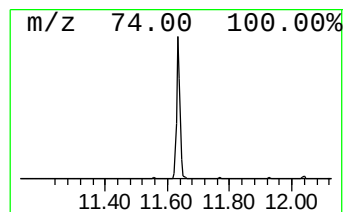
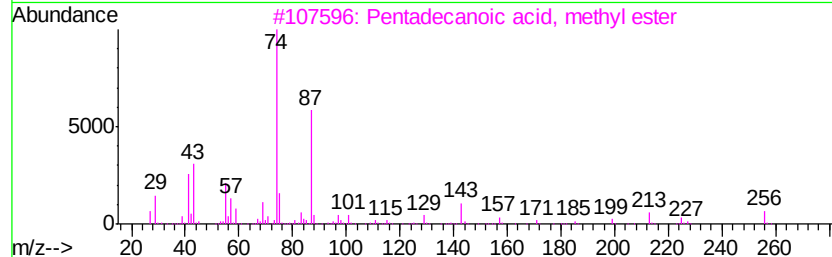
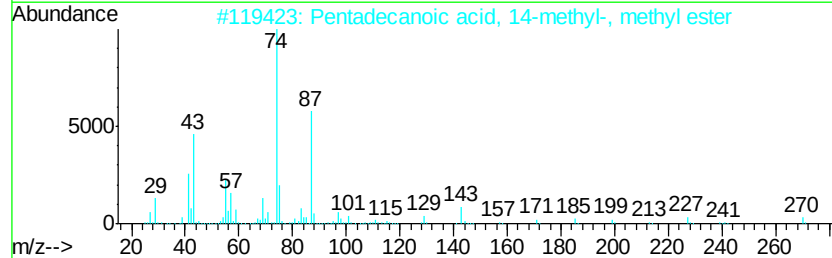
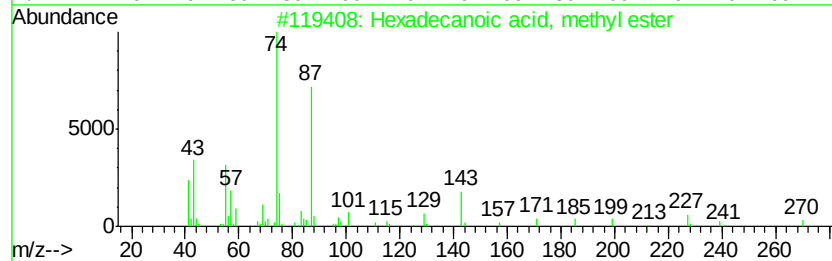
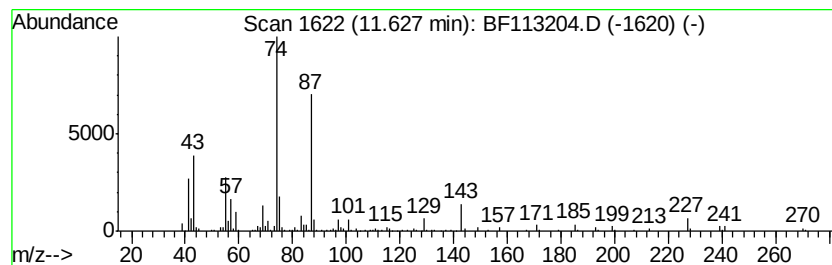
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.63	10.83 ng	751389	Phenanthrene-d10	11.23		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	99
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3		Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
5		Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	80



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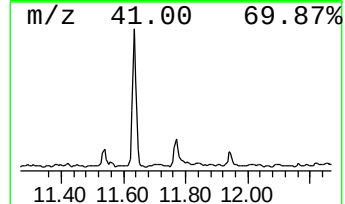
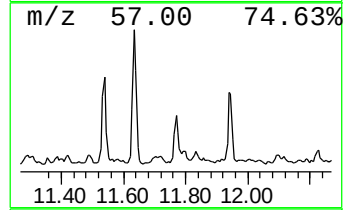
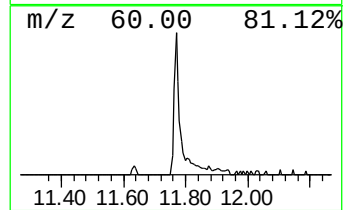
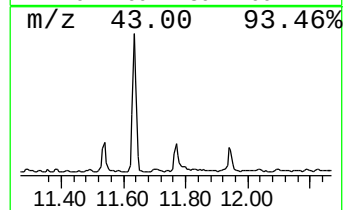
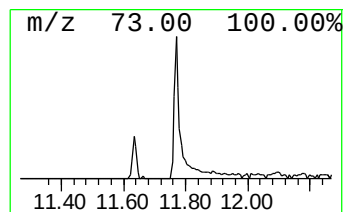
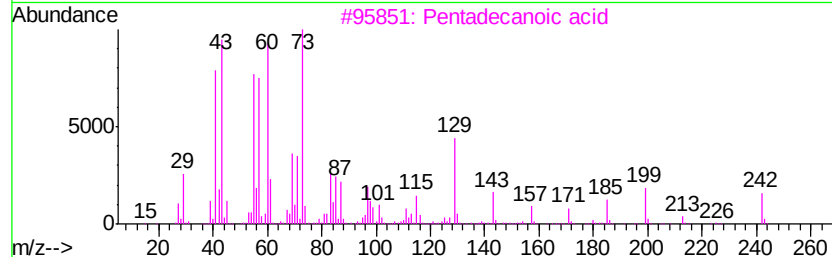
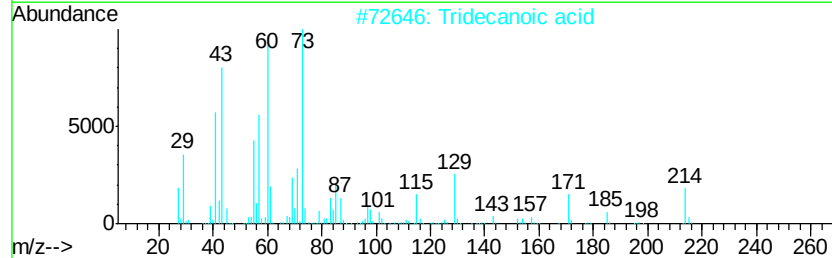
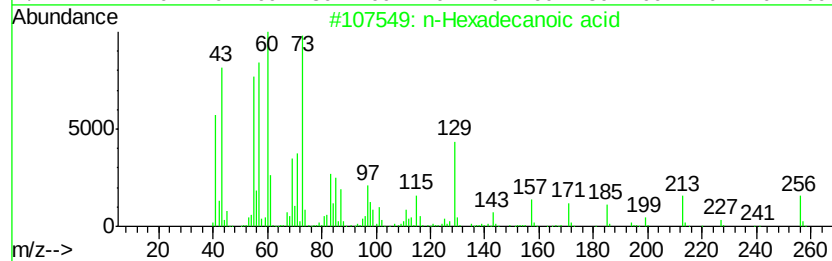
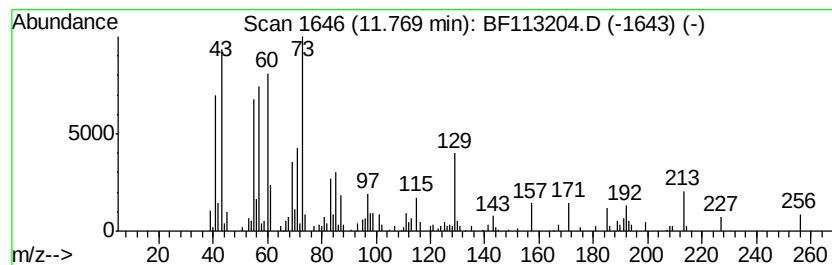
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	2.65 ng	184069	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		Undecanoic acid	186	C11H22O2	000112-37-8	38



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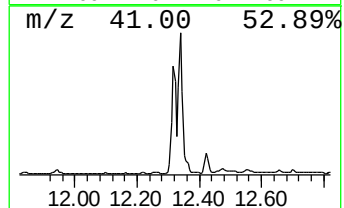
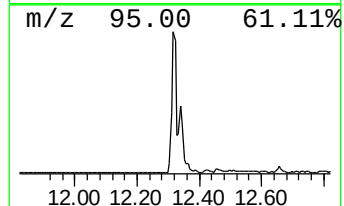
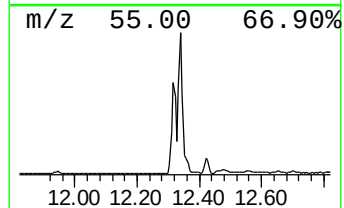
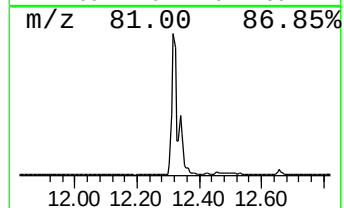
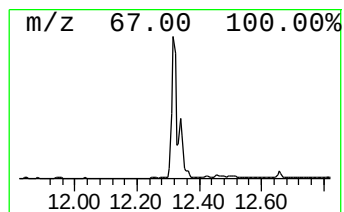
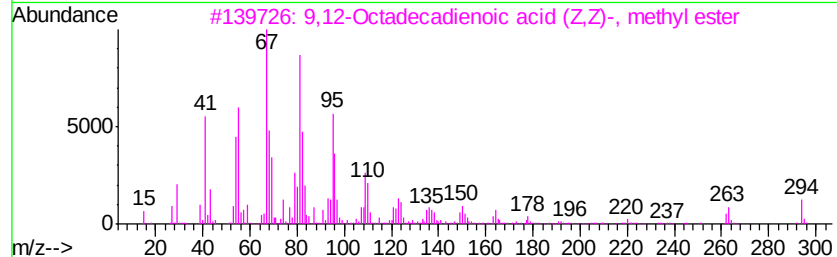
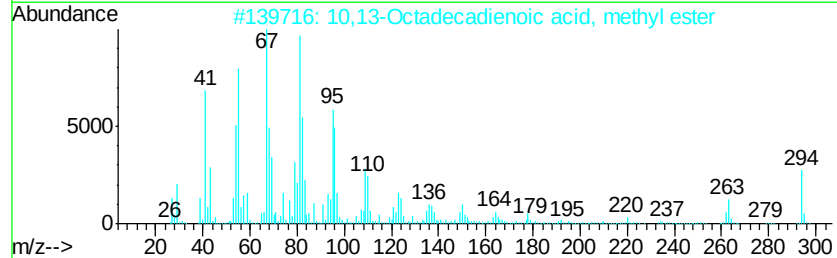
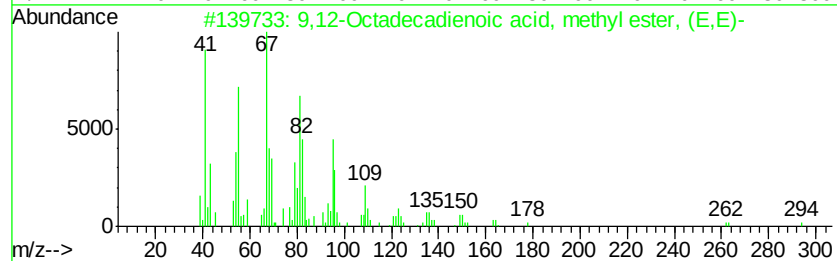
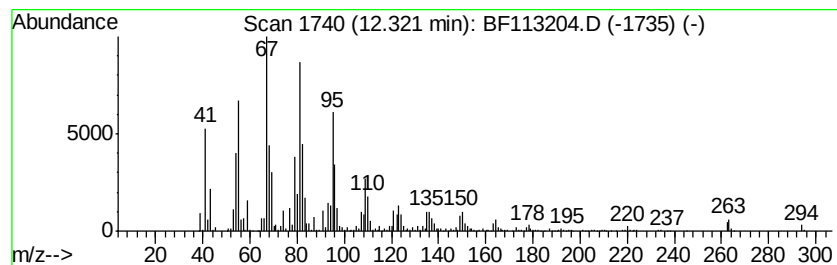
Instrument :
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ClientSampleId :
JC-02-031919-G

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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 9,12-Octadecadienoic acid, ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.32	34.94 ng	2424670	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
2	10,13-Octadecadienoic acid, meth...	294	C19H34O2	056554-62-2	99
3	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
4	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
5	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113204.D
Acq On : 21 Mar 2019 13:11
Operator : JU/SJ
Sample : K1688-33 10X
Misc :
ALS Vial : 7 Sample Multiplier: 1

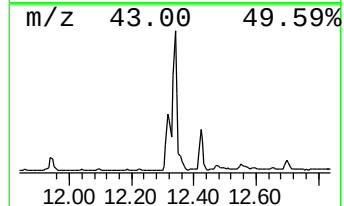
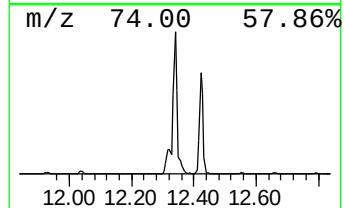
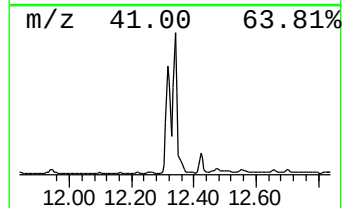
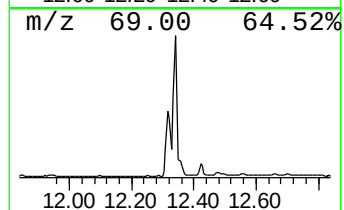
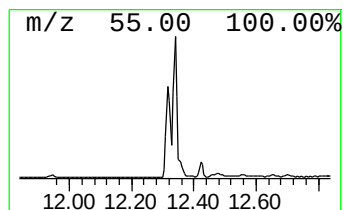
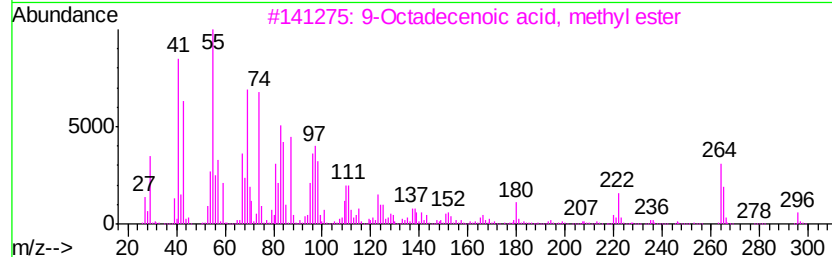
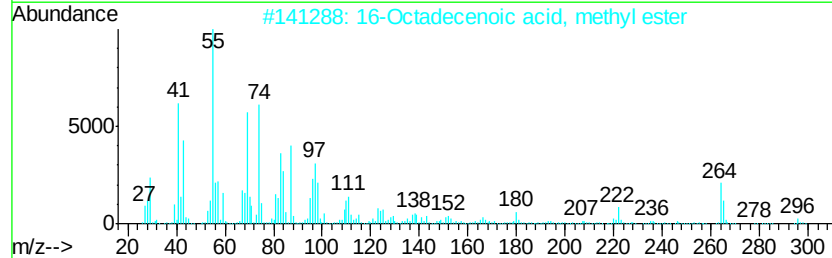
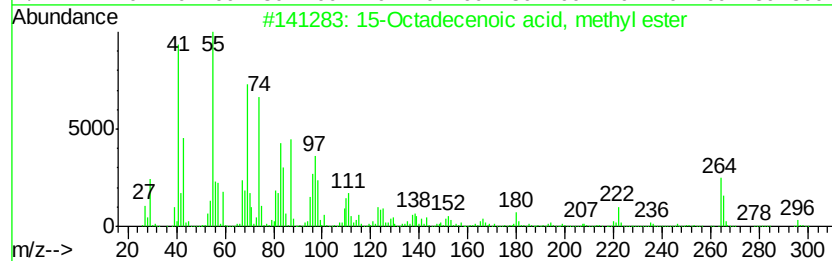
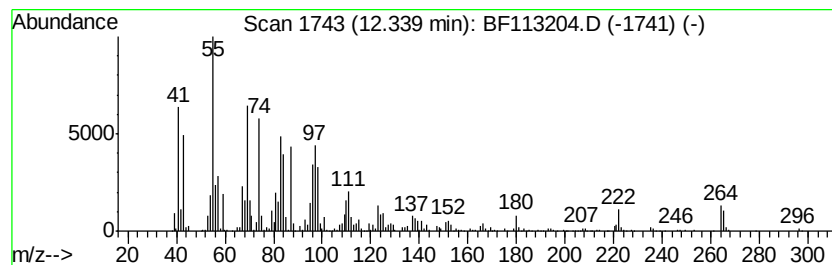
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 15-Octadecenoic acid, methyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.34	32.35 ng	2245000	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
2	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	99
3	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
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Sample : K1688-33 10X
Misc :
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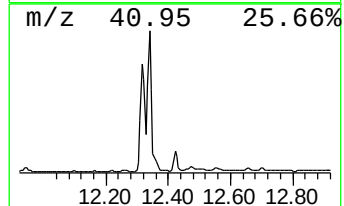
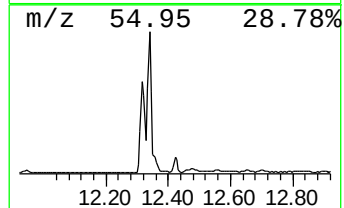
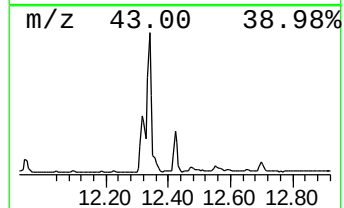
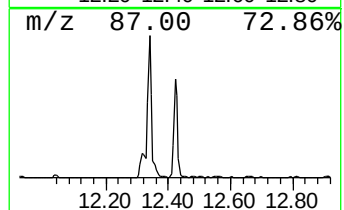
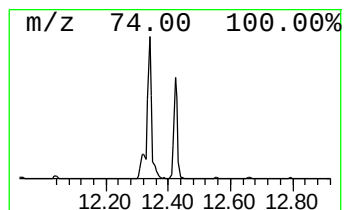
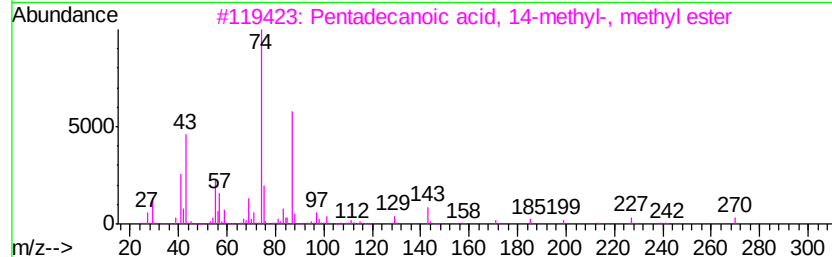
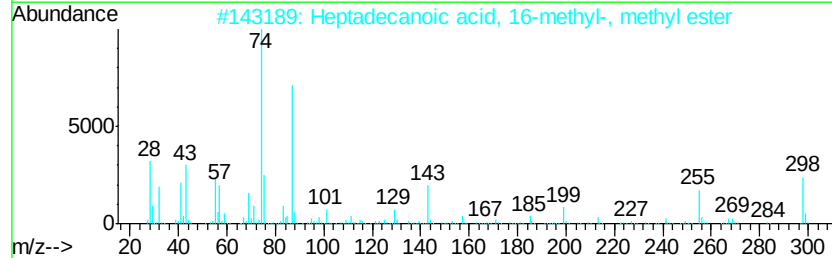
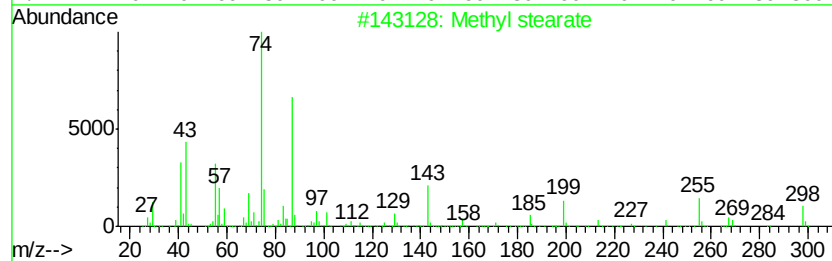
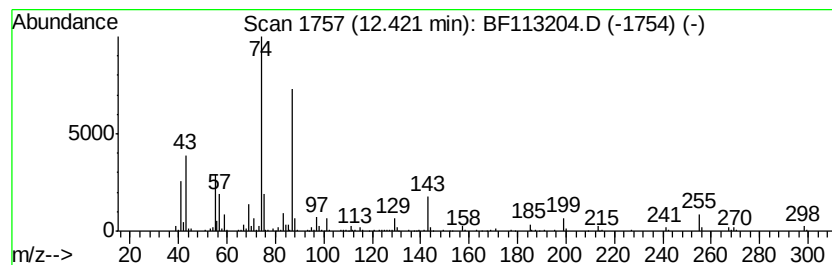
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.42	5.70 ng	395452	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	98
2	Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	95
3	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
4	Methyl tetradecanoate	242	C15H30O2	000124-10-7	93
5	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113204.D
Acq On : 21 Mar 2019 13:11
Operator : JU/SJ
Sample : K1688-33 10X
Misc :
ALS Vial : 7 Sample Multiplier: 1

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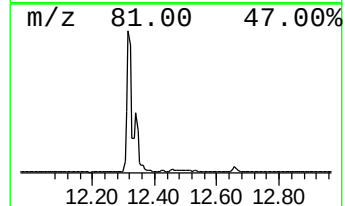
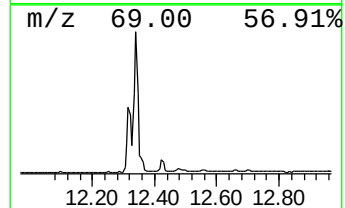
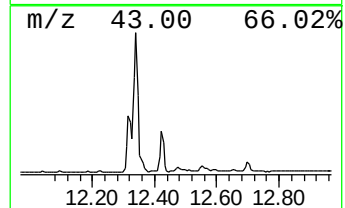
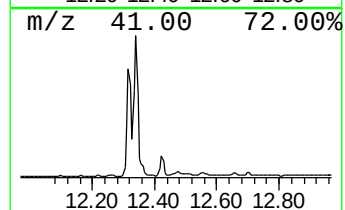
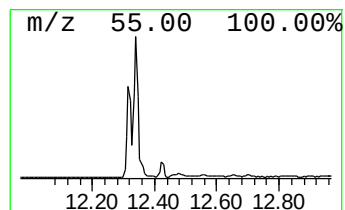
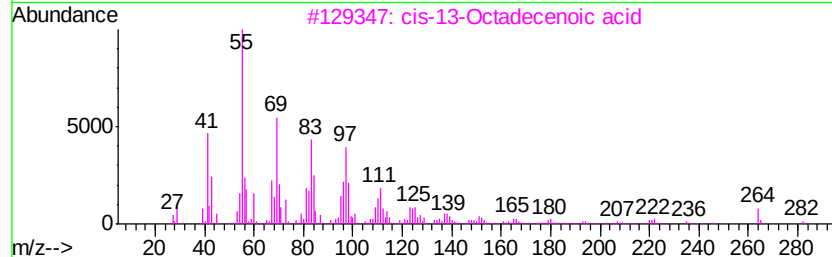
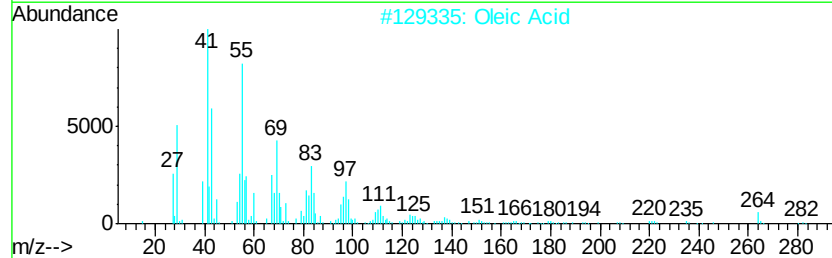
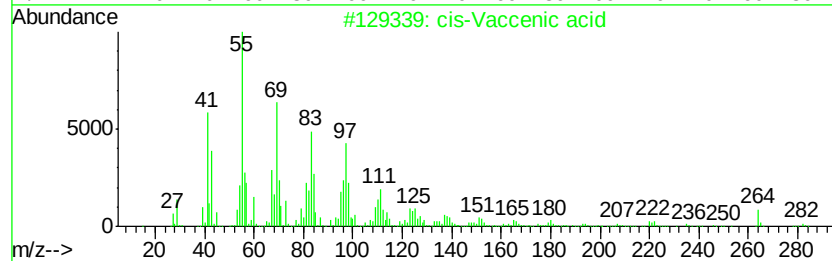
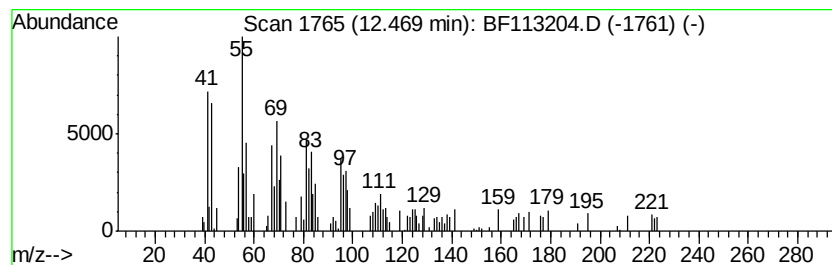
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 cis-Vaccenic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.47	2.46 ng	170661	Phenanthrene-d10	11.23

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		cis-Vaccenic acid	282	C18H34O2	000506-17-2	93
2		Oleic Acid	282	C18H34O2	000112-80-1	83
3		cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	74
4		9-octadecenoic acid, 2,2,2-trifl...	364	C20H35F3O2	1000376-54-3	72
5		9-octadecanoic acid, 2,2,3,3,4,4...	464	C22H35F7O2	1000376-61-4	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
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Sample : K1688-33 10X
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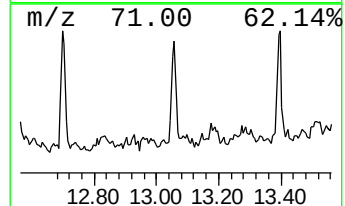
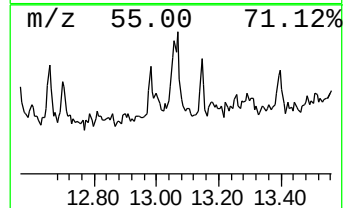
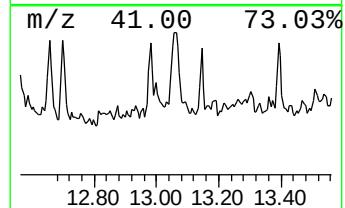
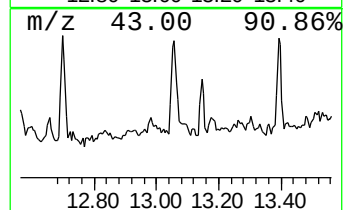
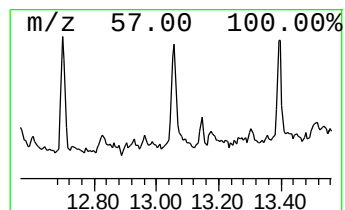
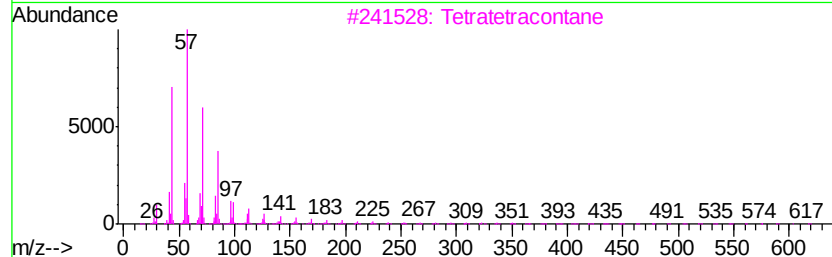
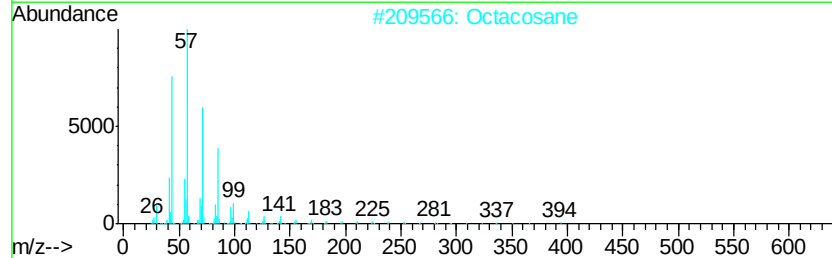
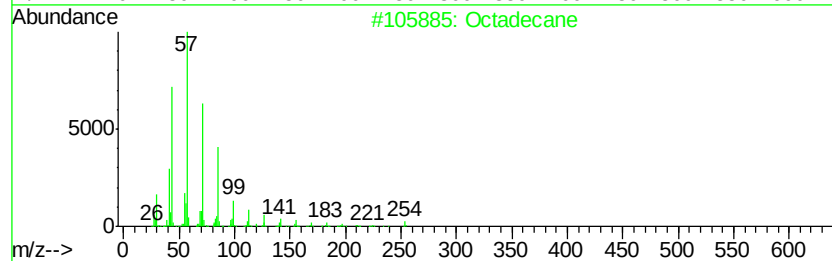
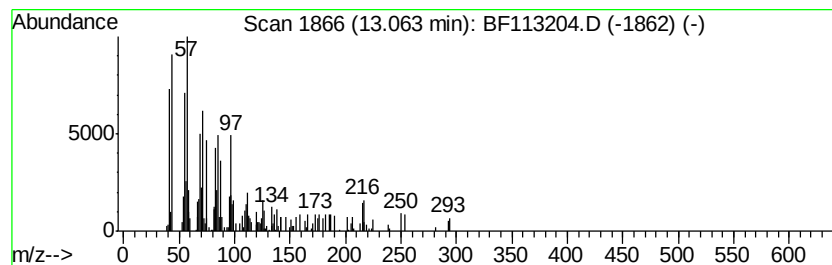
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.06	2.11 ng	114579	Chrysene-d12	13.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254 C18H38	000593-45-3	89
2	Octacosane	394 C28H58	000630-02-4	68
3	Tetratetracontane	619 C44H90	007098-22-8	68
4	Heneicosane	296 C21H44	000629-94-7	68
5	Heptacosane	380 C27H56	000593-49-7	68



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113204.D
Acq On : 21 Mar 2019 13:11
Operator : JU/SJ
Sample : K1688-33 10X
Misc :
ALS Vial : 7 Sample Multiplier: 1

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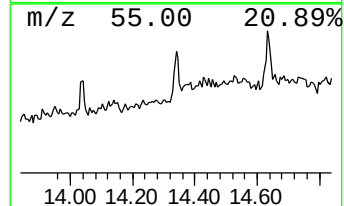
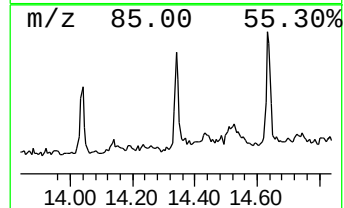
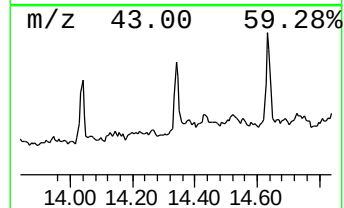
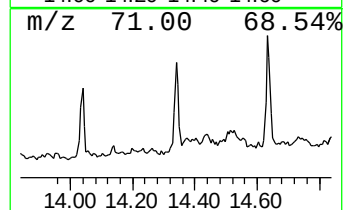
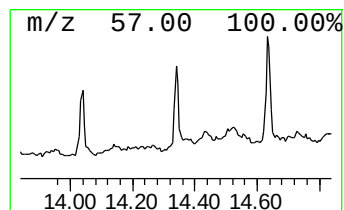
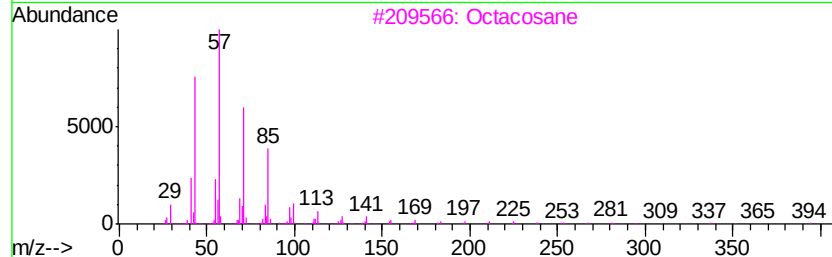
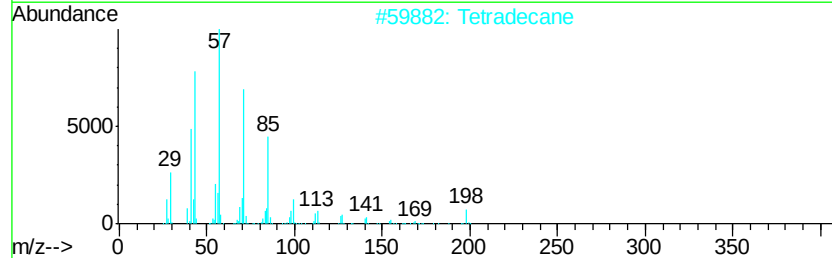
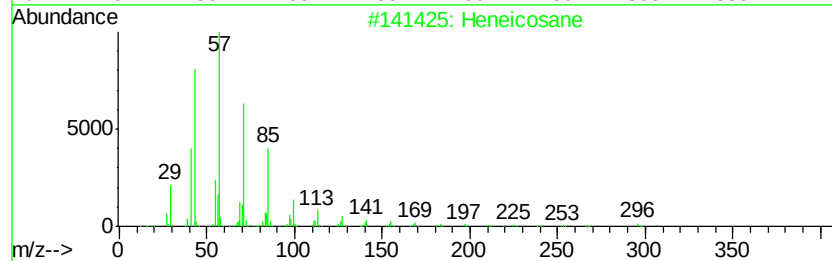
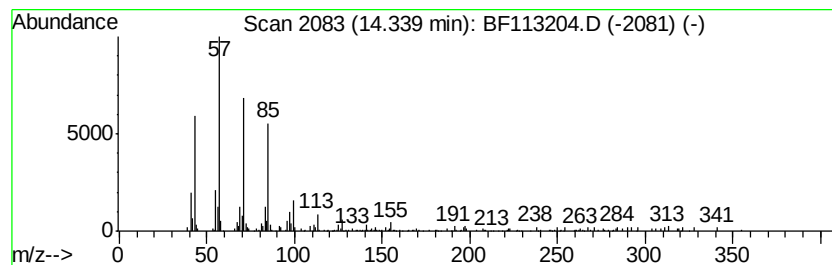
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heneicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	2.05 ng	111511	Chrysene-d12	13.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Tetradecane	198	C14H30	000629-59-4	83
3		Octacosane	394	C28H58	000630-02-4	64
4		Heptacosane	380	C27H56	000593-49-7	64
5		Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
 Data File : BF113204.D
 Acq On : 21 Mar 2019 13:11
 Operator : JU/SJ
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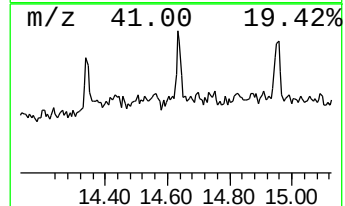
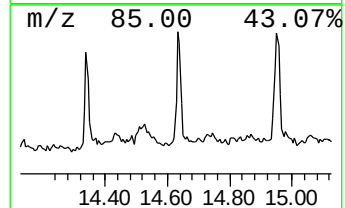
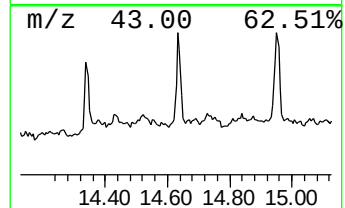
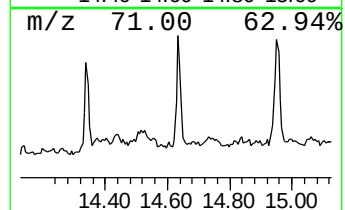
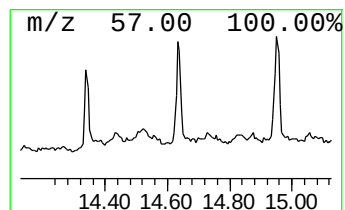
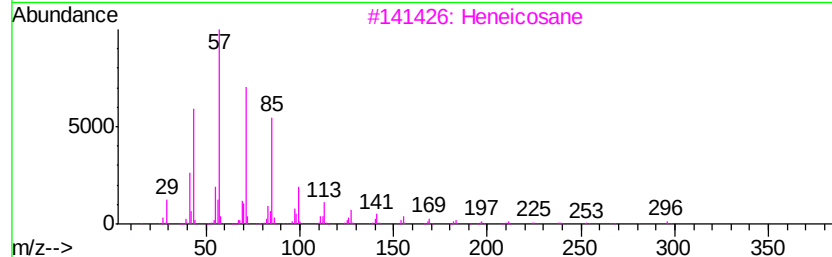
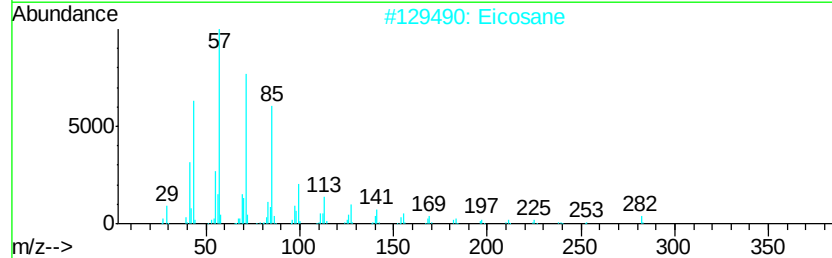
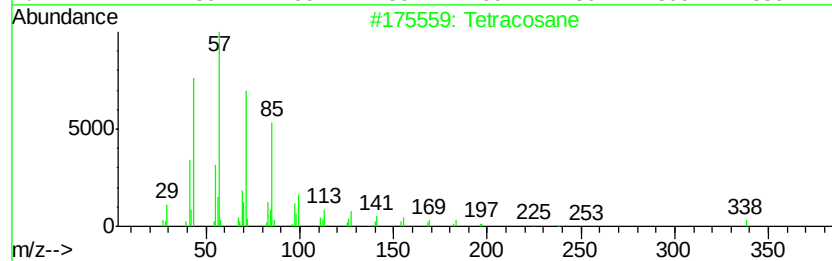
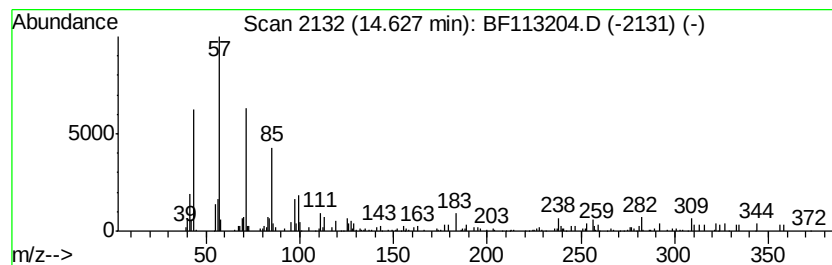
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 12 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	2.39 ng	134904	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tetracosane	338	C24H50	000646-31-1	93
2		Eicosane	282	C20H42	000112-95-8	93
3		Heneicosane	296	C21H44	000629-94-7	90
4		Heptadecane	240	C17H36	000629-78-7	87
5		Nonadecane	268	C19H40	000629-92-5	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113204.D
Acq On : 21 Mar 2019 13:11
Operator : JU/SJ
Sample : K1688-33 10X
Misc :
ALS Vial : 7 Sample Multiplier: 1

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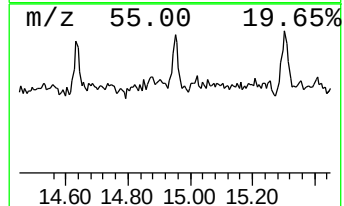
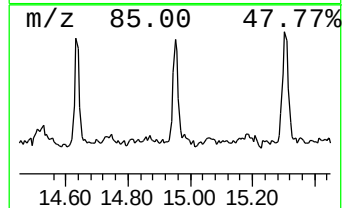
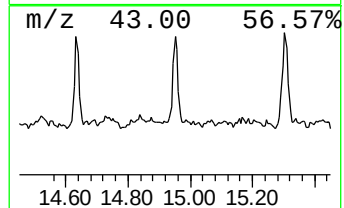
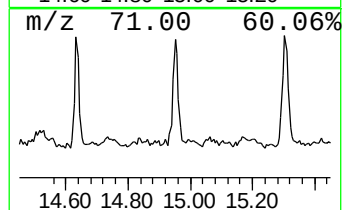
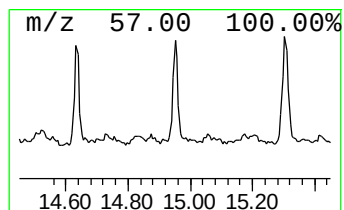
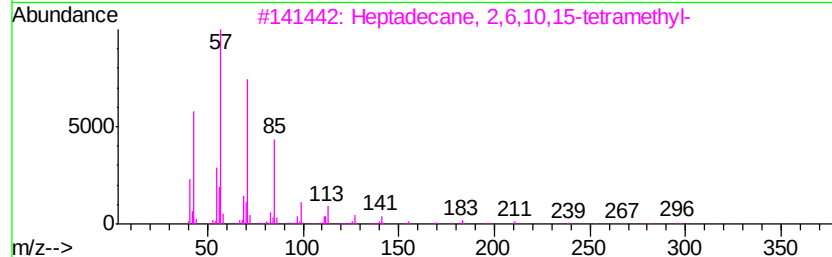
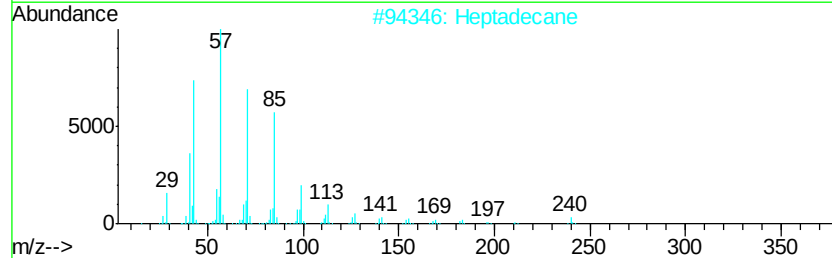
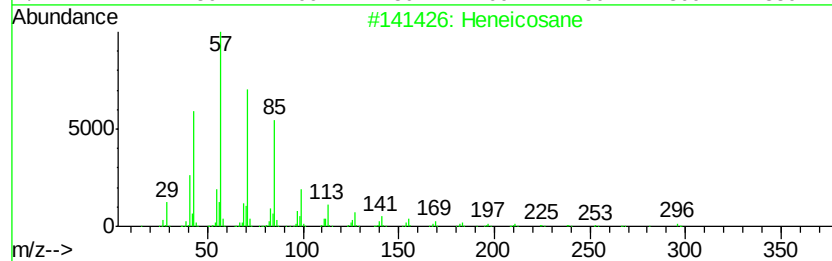
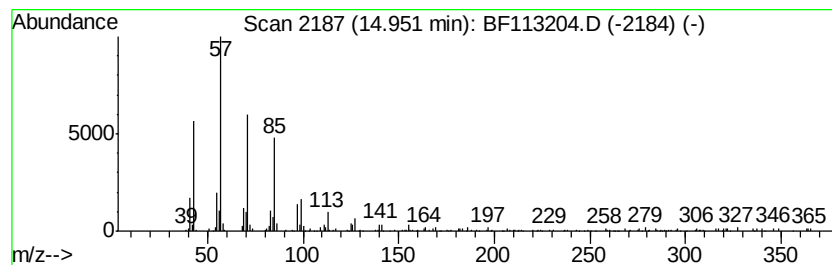
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	3.05 ng	172681	Perylene-d12	15.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	98
2		Heptadecane	240	C17H36	000629-78-7	87
3		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4		Hentriacontane	437	C31H64	000630-04-6	86
5		Hexadecane	226	C16H34	000544-76-3	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
Data File : BF113204.D
Acq On : 21 Mar 2019 13:11
Operator : JU/SJ
Sample : K1688-33 10X
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
JC-02-031919-G

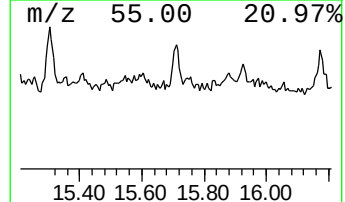
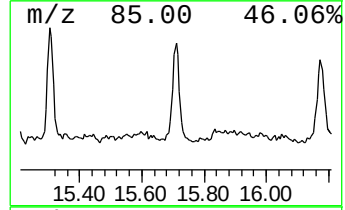
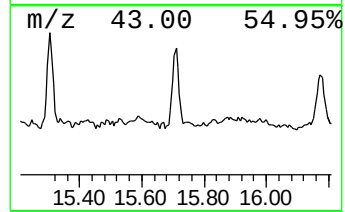
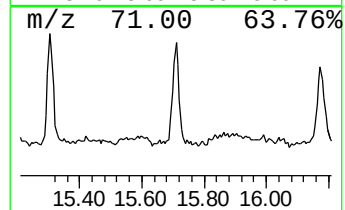
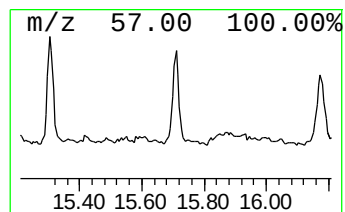
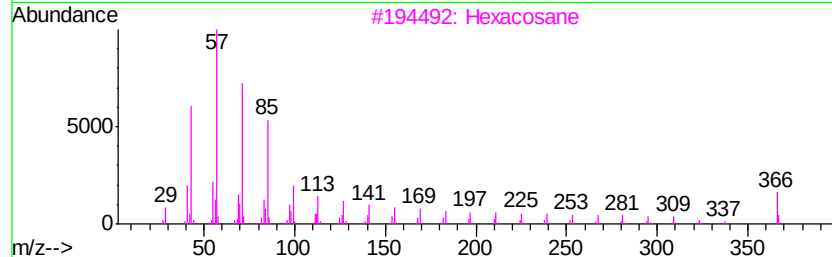
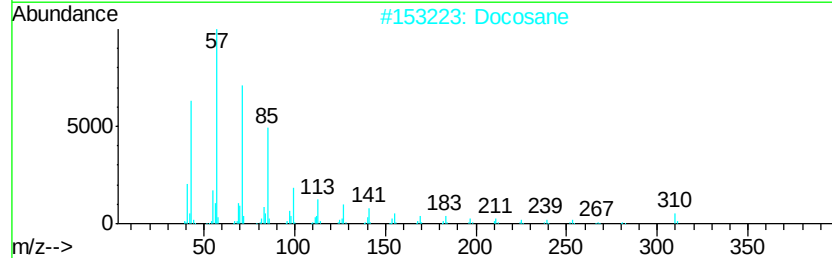
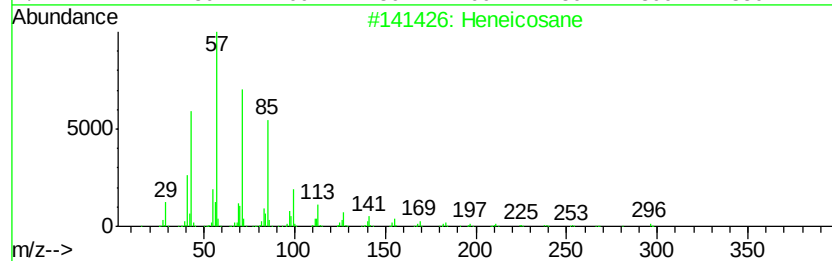
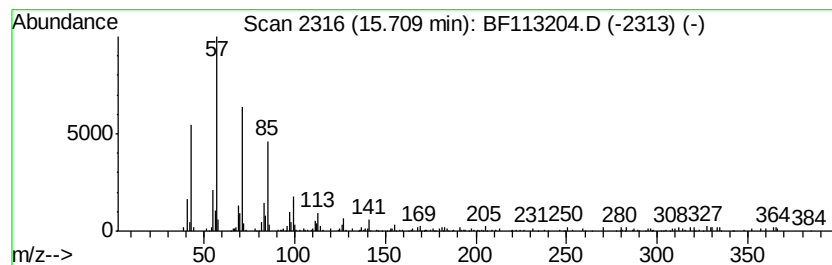
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	2.52 ng	142229	Perylene-d12	15.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	99
2			Docosane	310	C22H46	000629-97-0	97
3			Hexacosane	366	C26H54	000630-01-3	91
4			2-methyloctacosane	408	C29H60	1000376-72-8	91
5			Tridecane, 6-propyl-	226	C16H34	055045-10-8	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF032119\
 Data File : BF113204.D
 Acq On : 21 Mar 2019 13:11
 Operator : JU/SJ
 Sample : K1688-33 10X
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 JC-02-031919-G

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF022719.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
unknown6.49	6.49	6.8 ng		287018	1	6.72	841273	20.0
Tridecane	10.66	2.1 ng		145013	4	11.23	1388090	20.0
Hexadecanoic acid...	11.63	10.8 ng		751389	4	11.23	1388090	20.0
n-Hexadecanoic acid	11.77	2.6 ng		184069	4	11.23	1388090	20.0
9,12-Octadecadien...	12.32	34.9 ng		2424670	4	11.23	1388090	20.0
15-Octadecenoic a...	12.34	32.4 ng		2245000	4	11.23	1388090	20.0
Methyl stearate	12.42	5.7 ng		395452	4	11.23	1388090	20.0
cis-Vaccenic acid	12.47	2.5 ng		170661	4	11.23	1388090	20.0
Octadecane	13.06	2.1 ng		114579	5	13.86	1087080	20.0
Heneicosane	14.34	2.0 ng		111511	5	13.86	1087080	20.0
Tetracosane	14.63	2.4 ng		134904	6	15.27	1130990	20.0
Heptadecane	14.95	3.0 ng		172681	6	15.27	1130990	20.0
Hexacosane	15.71	2.5 ng		142229	6	15.27	1130990	20.0