

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
 Data File : BF107758.D
 Acq On : 27 Jul 2018 20:49
 Operator : JU/SJ
 Sample : J4121-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GW-03(8-10)

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-BF072018.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	4.101	294	300	307	rBV	48293	86357	2.31%	0.229%
2	5.201	482	487	499	rBV	427026	620906	16.58%	1.646%
3	5.454	527	530	539	rVB	33669	41000	1.09%	0.109%
4	5.560	545	548	550	rBV	53261	69097	1.84%	0.183%
5	5.595	550	554	576	rVV	2310774	3115640	83.18%	8.261%
6	5.813	588	591	597	rVB2	37402	43145	1.15%	0.114%
7	6.595	720	724	744	rBV	2105760	3467874	92.58%	9.195%
8	6.736	744	748	771	rVB	2866991	3745693	100.00%	9.931%
9	6.960	783	786	806	rBV	656858	975483	26.04%	2.586%
10	7.113	808	812	827	rVV	2410314	2807813	74.96%	7.445%
11	7.219	827	830	843	rVB	94328	176657	4.72%	0.468%
12	7.525	878	882	906	rBV	1506429	2297178	61.33%	6.091%
13	8.242	1000	1004	1015	rBV	1043838	1278730	34.14%	3.390%
14	9.313	1180	1186	1195	rBV	3160159	3330883	88.93%	8.831%
15	9.707	1247	1253	1263	rBV	204128	216009	5.77%	0.573%
16	10.001	1299	1303	1320	rVB	1186195	1261522	33.68%	3.345%
17	10.407	1364	1372	1376	rBV2	42978	59922	1.60%	0.159%
18	10.795	1434	1438	1450	rBV	1939889	2260463	60.35%	5.993%
19	10.883	1450	1453	1458	rVB2	48939	74236	1.98%	0.197%
20	11.495	1553	1557	1560	rBV	1028368	1093954	29.21%	2.901%
21	11.519	1560	1561	1568	rVV	289345	276697	7.39%	0.734%
22	11.571	1568	1570	1578	rVB	74498	112052	2.99%	0.297%
23	11.860	1616	1619	1624	rBV	245913	212901	5.68%	0.564%
24	12.001	1639	1643	1645	rBV2	224553	216450	5.78%	0.574%
25	12.024	1645	1647	1653	rVB3	71929	85135	2.27%	0.226%
26	12.113	1658	1662	1664	rBV2	102988	125288	3.34%	0.332%
27	12.166	1669	1671	1675	rBV2	35768	39288	1.05%	0.104%
28	12.289	1690	1692	1695	rBV2	38520	43099	1.15%	0.114%
29	12.518	1728	1731	1734	rBV	175067	181340	4.84%	0.481%
30	12.554	1734	1737	1738	rVV2	185849	191250	5.11%	0.507%
31	12.571	1738	1740	1749	rVV	536244	662197	17.68%	1.756%
32	12.654	1752	1754	1761	rVV	130870	125039	3.34%	0.332%
33	12.718	1762	1765	1772	rVB	556922	528915	14.12%	1.402%
34	12.942	1797	1803	1809	rBV	385826	535834	14.31%	1.421%

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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	13.077	1822	1826	1836	rVB	2402192	2417603	64.54%	6.410%
36	13.271	1856	1859	1864	rVB3	117969	163191	4.36%	0.433%
37	13.336	1867	1870	1873	rBV	77095	78276	2.09%	0.208%
38	13.507	1896	1899	1902	rVB3	96759	91142	2.43%	0.242%
39	13.624	1916	1919	1922	rBV2	86660	98066	2.62%	0.260%
40	13.954	1972	1975	1981	rVB3	297163	304281	8.12%	0.807%
41	14.095	1997	1999	2003	rBV2	56557	56078	1.50%	0.149%
42	14.148	2003	2008	2011	rBV2	1069588	1462696	39.05%	3.878%
43	14.271	2027	2029	2031	rBV	69584	55114	1.47%	0.146%
44	14.895	2133	2135	2139	rVB	90310	86863	2.32%	0.230%
45	15.224	2187	2191	2193	rBV	144203	219316	5.86%	0.581%
46	15.248	2193	2195	2202	rVB3	157271	221308	5.91%	0.587%
47	15.542	2243	2245	2251	rBV	60873	64955	1.73%	0.172%
48	15.612	2253	2257	2260	rVV	177513	288312	7.70%	0.764%
49	15.677	2264	2268	2291	rVB	703600	1750794	46.74%	4.642%

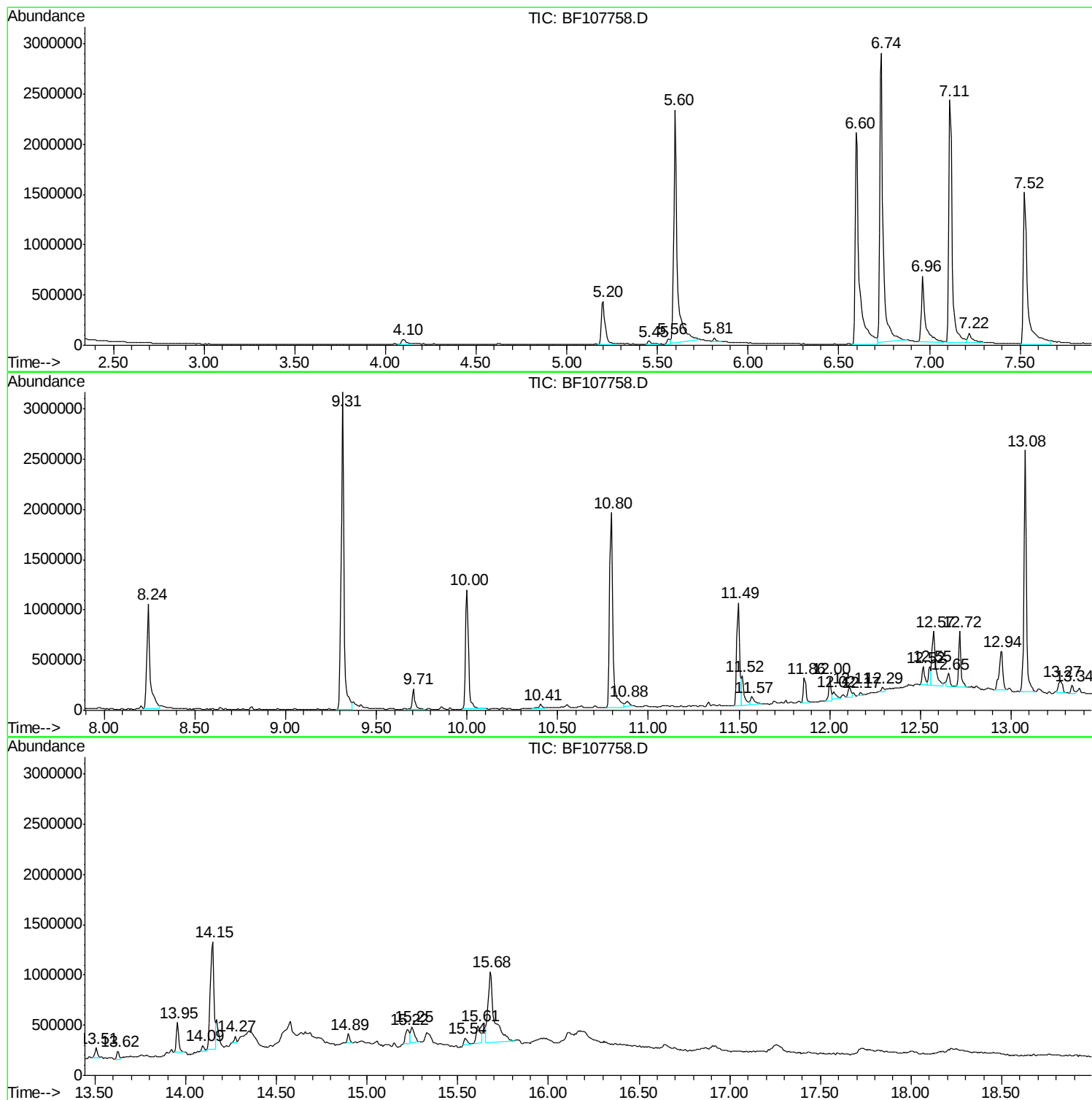
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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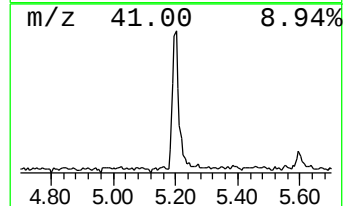
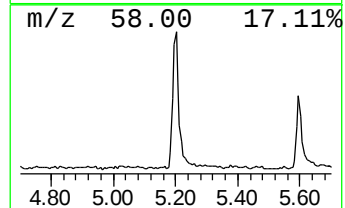
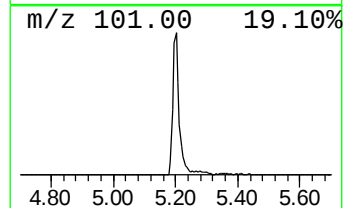
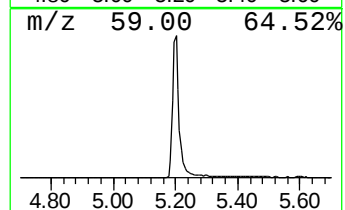
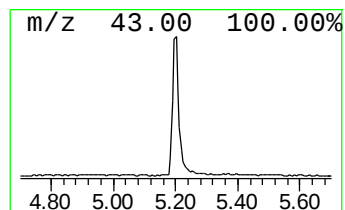
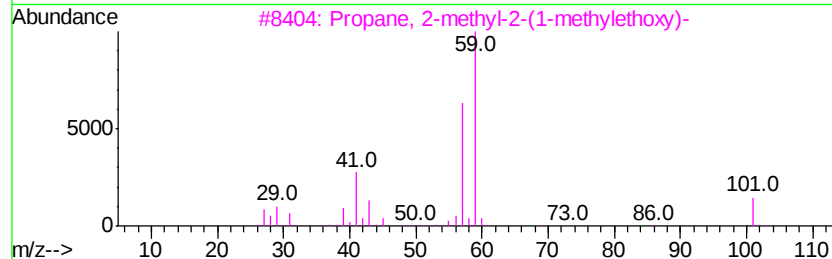
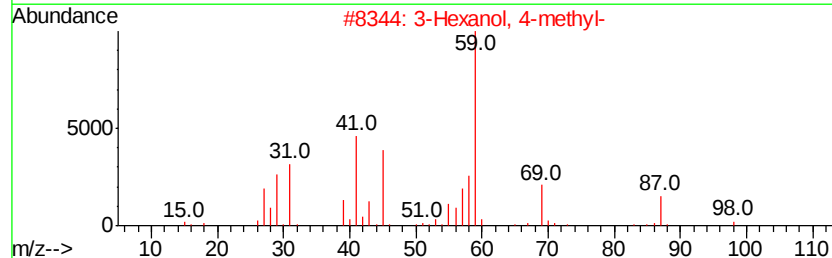
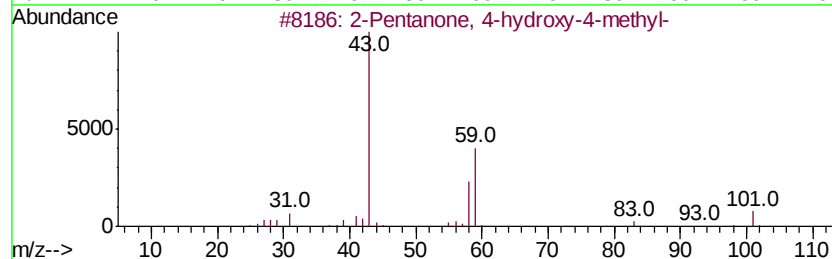
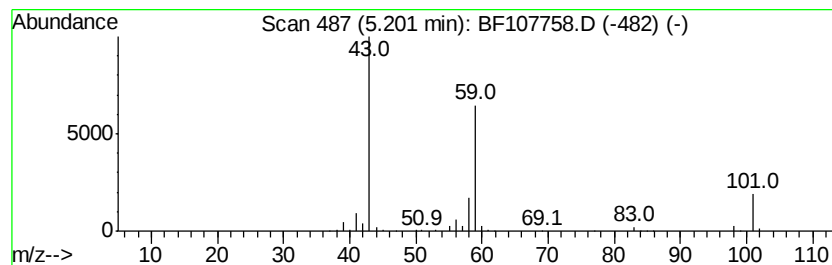
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	12.73 ng	620906	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	28
4			Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	17
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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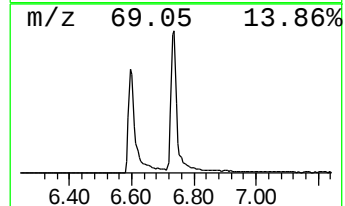
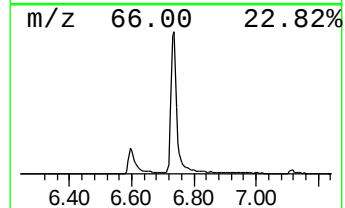
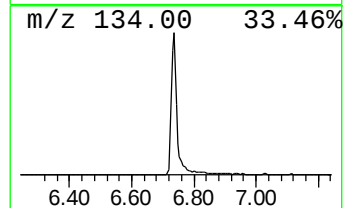
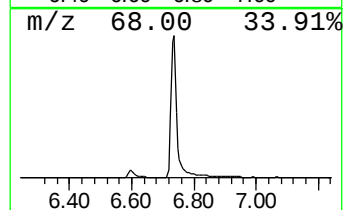
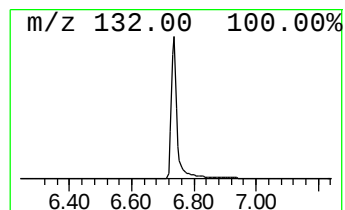
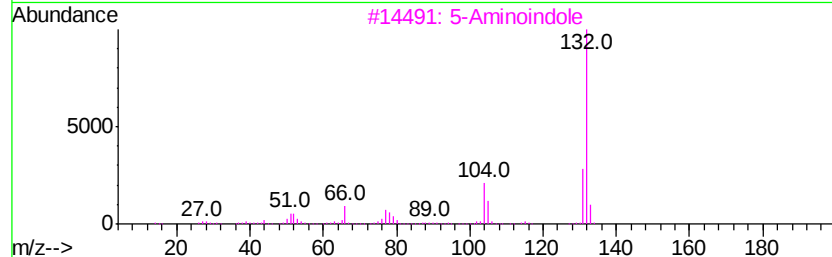
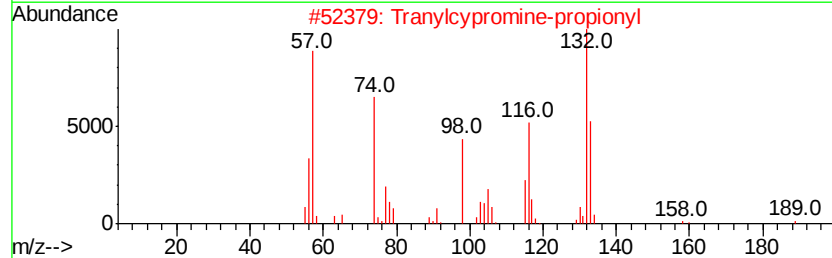
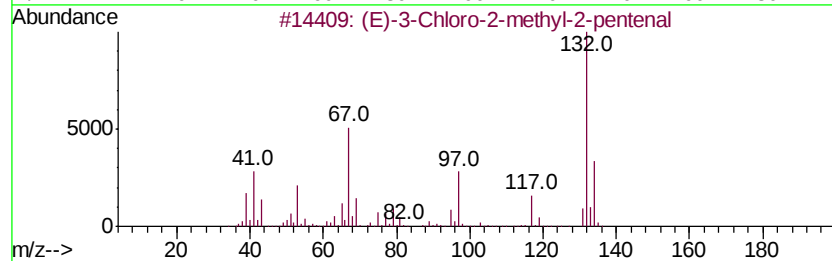
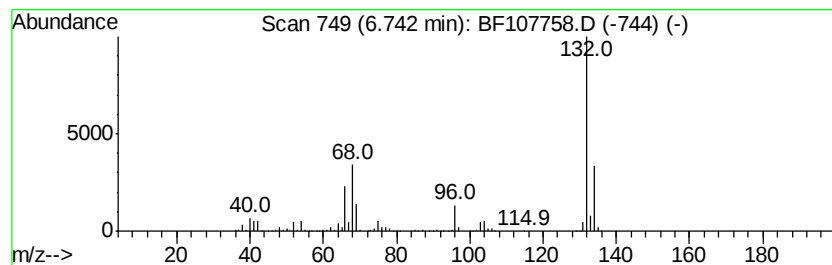
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	76.80 ng	3745690	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9



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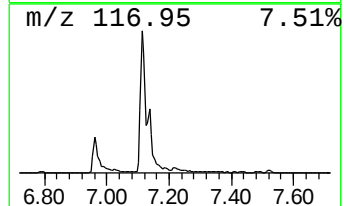
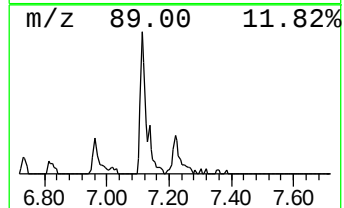
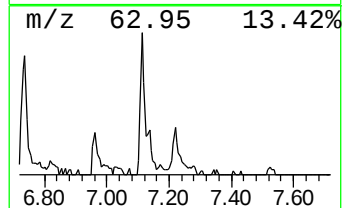
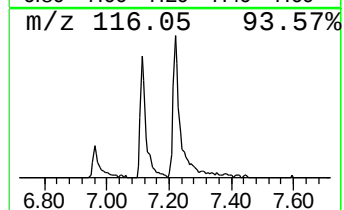
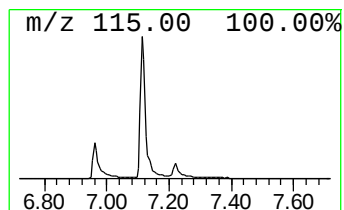
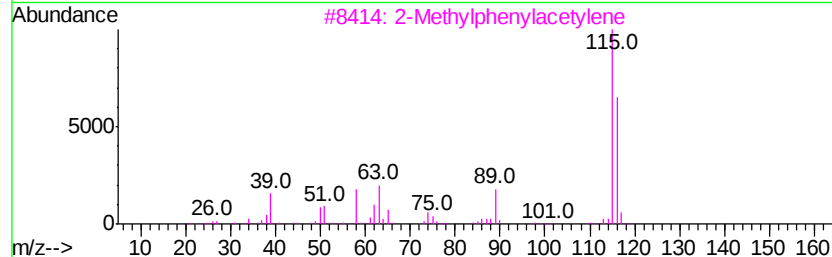
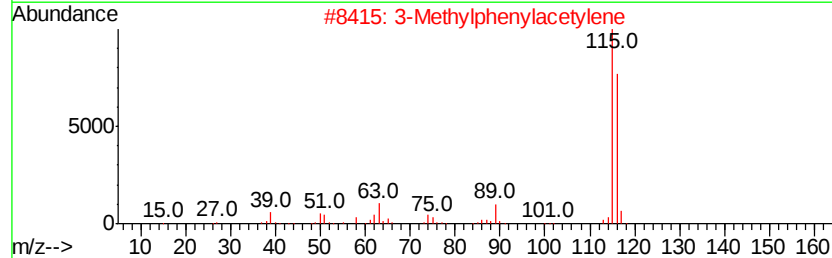
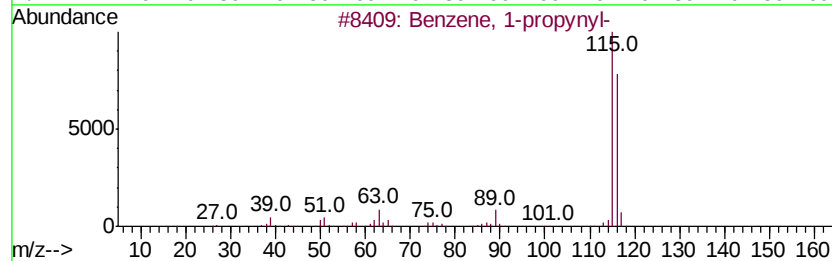
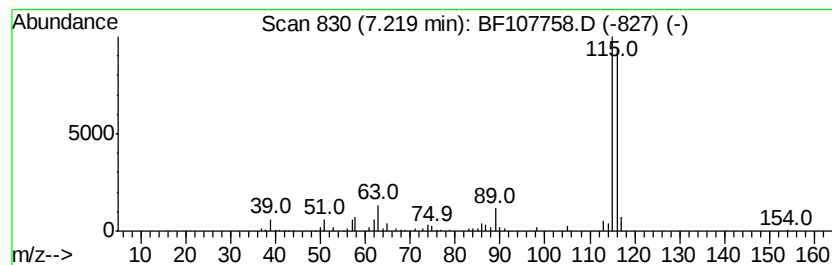
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-propynyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	3.62 ng	176657	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
2		3-Methylphenylacetylene	116	C9H8	000766-82-5	91
3		2-Methylphenylacetylene	116	C9H8	000766-47-2	90
4		Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	87
5		1-Propyne, 3-phenyl-	116	C9H8	010147-11-2	78



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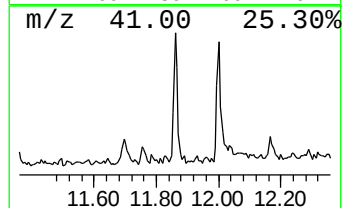
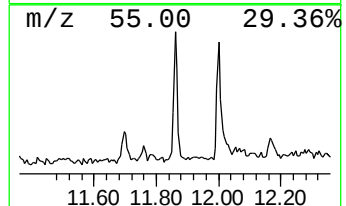
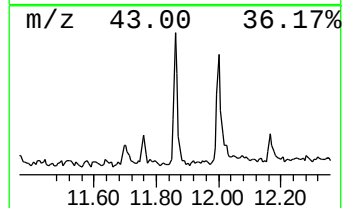
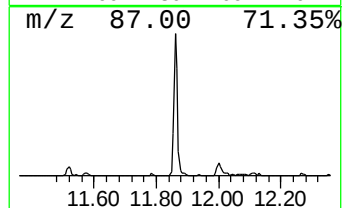
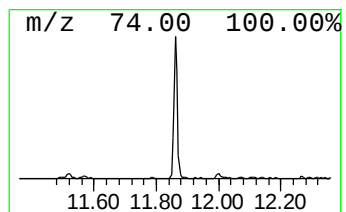
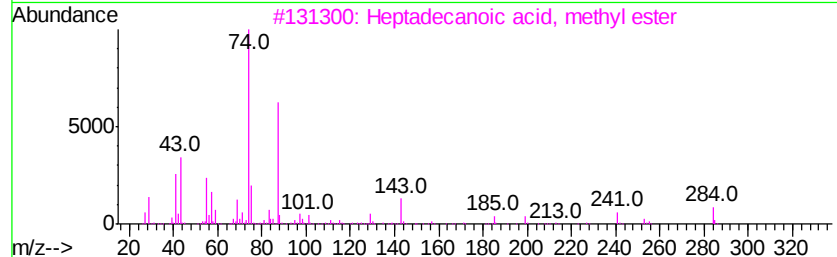
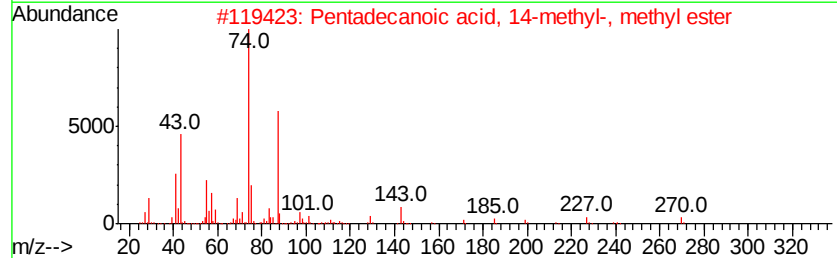
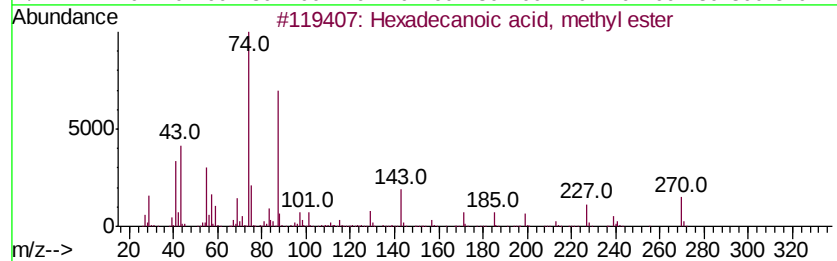
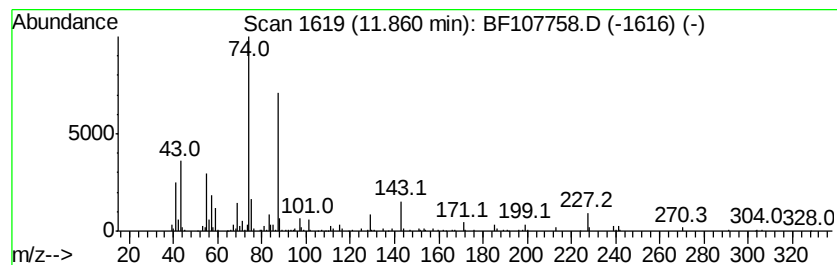
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	3.89 ng	212901	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	93
2		Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	90
3		Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	87
4		Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5		Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	86



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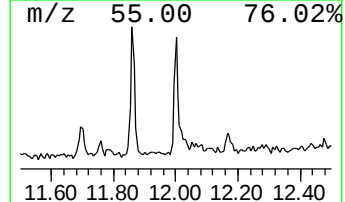
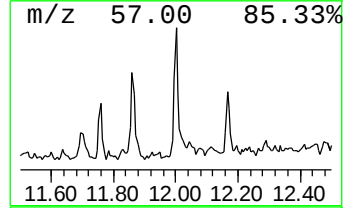
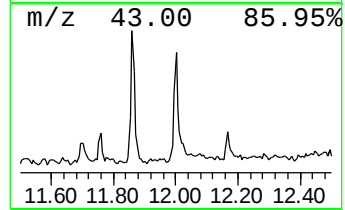
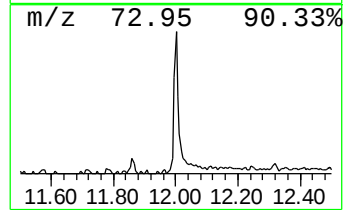
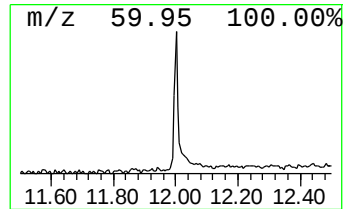
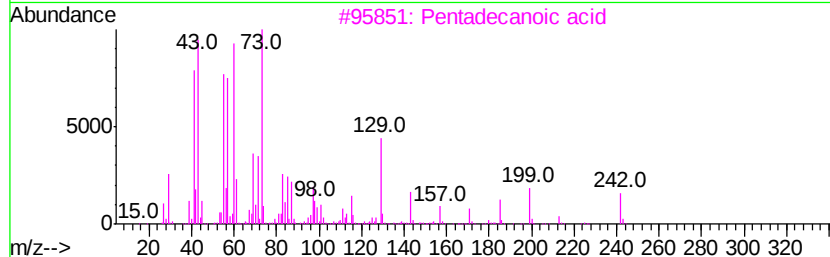
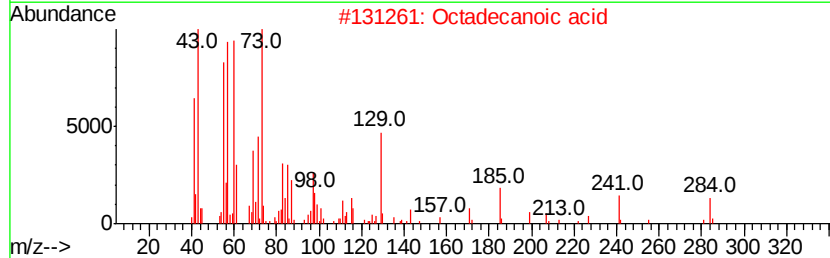
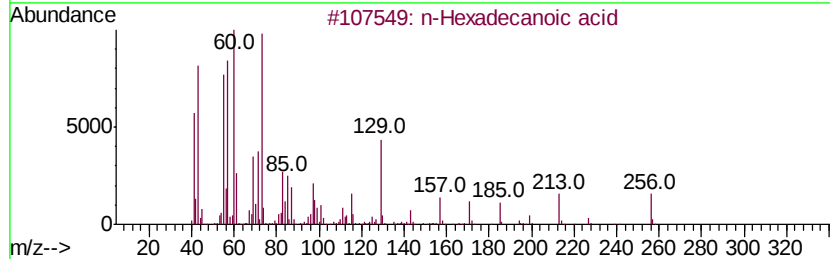
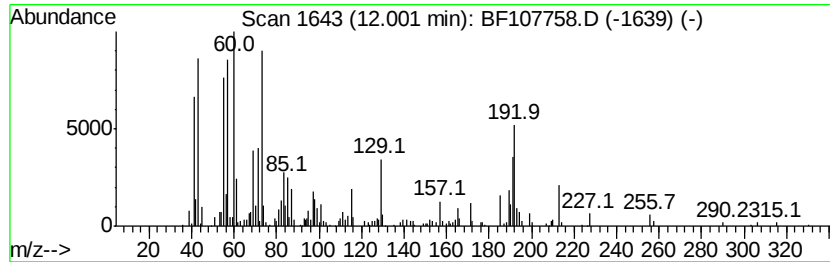
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.00	3.96 ng	216450	Phenanthrene-d10	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Octadecanoic acid	284	C18H36O2	000057-11-4	70
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	1H-Cyclopropa[1]phenanthrene,1a,...	192	C15H12	000949-41-7	53



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
Data File : BF107758.D
Acq On : 27 Jul 2018 20:49
Operator : JU/SJ
Sample : J4121-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

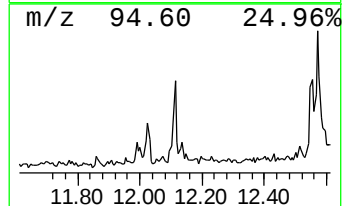
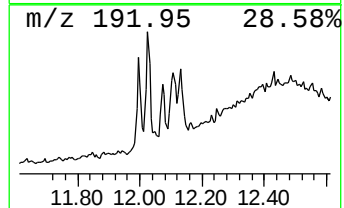
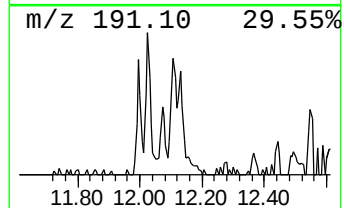
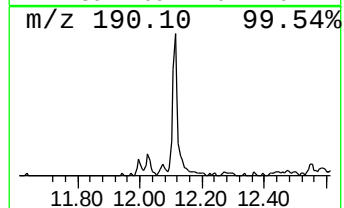
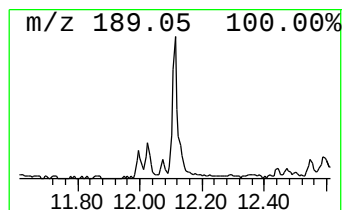
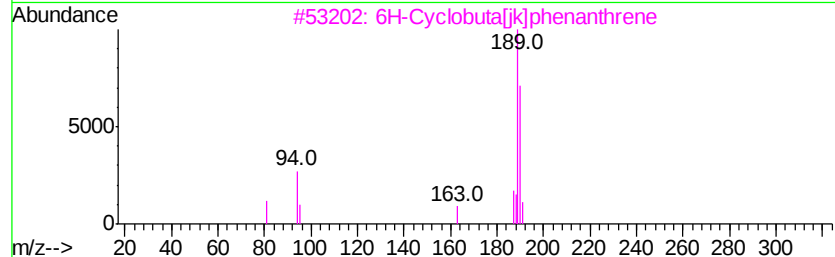
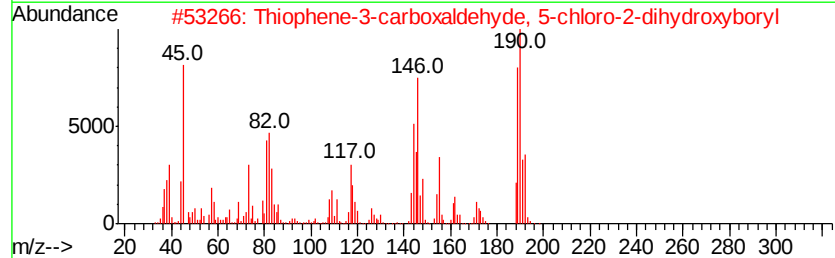
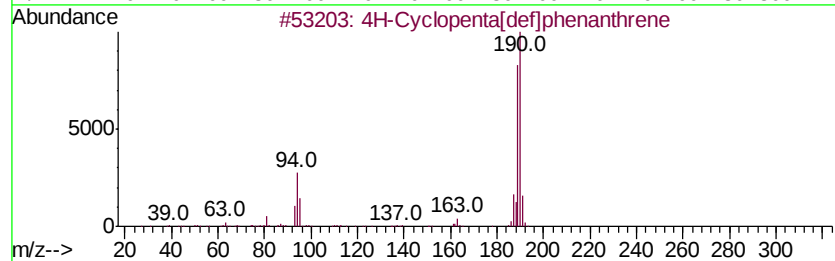
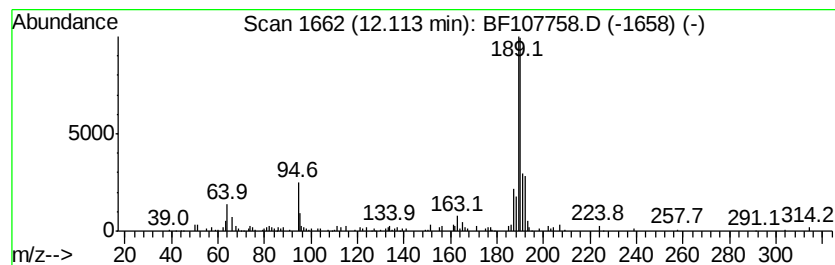
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.11	2.29 ng	125288	Phenanthrene-d10	11.49		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	80
2		Thiophene-3-carboxaldehyde, 5-ch...	190	C5H4BClO3S	036155-87-0	47
3		6H-Cyclobuta[flk]phenanthrene	190	C15H10	083469-43-6	42
4		2,2'-Bis(4,5-dimethylimidazole)	190	C10H14N4	069286-06-2	40
5		1,1'-Biphenyl,3,3'-difluoro-	190	C12H8F2	000396-64-5	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
Data File : BF107758.D
Acq On : 27 Jul 2018 20:49
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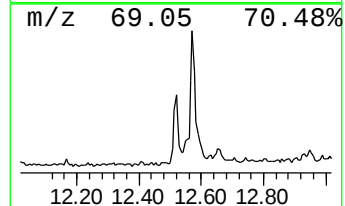
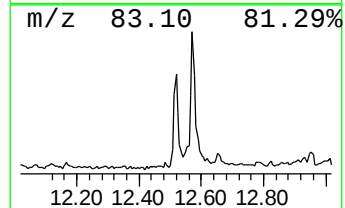
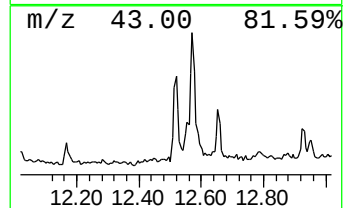
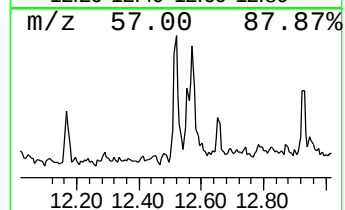
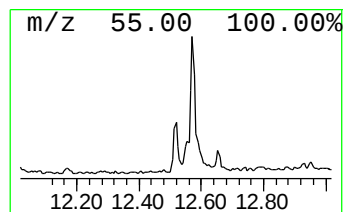
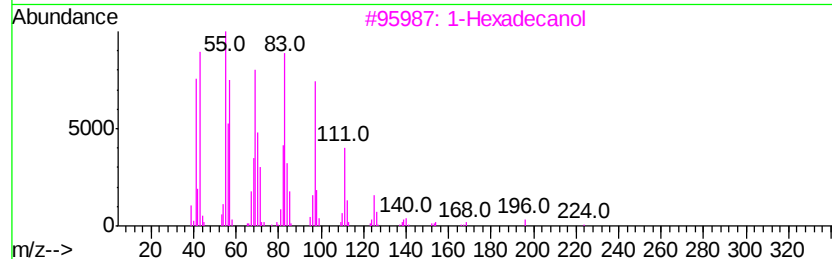
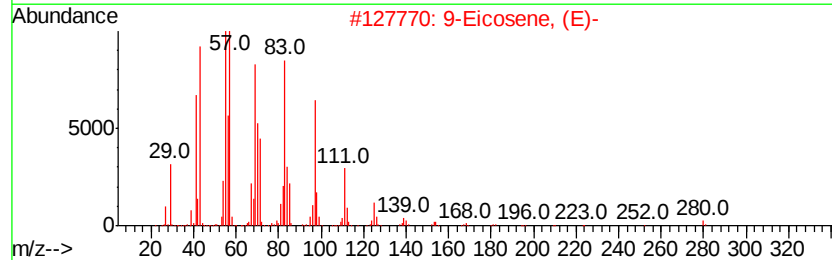
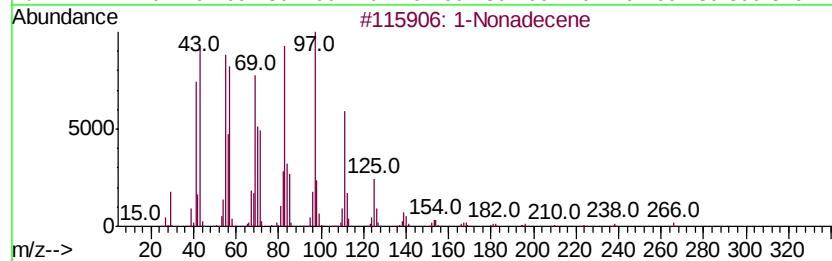
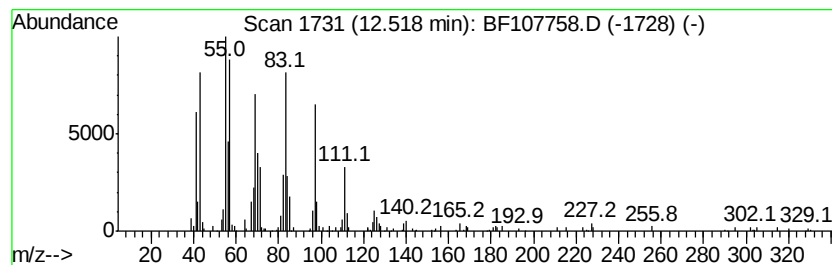
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Nonadecene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.52	3.32 ng	181340	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene		266	C19H38	018435-45-5	91
2	9-Eicosene, (E)-		280	C20H40	074685-29-3	91
3	1-Hexadecanol		242	C16H34O	036653-82-4	91
4	n-Nonadecanol-1		284	C19H40O	001454-84-8	91
5	5-Eicosene, (E)-		280	C20H40	074685-30-6	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
Data File : BF107758.D
Acq On : 27 Jul 2018 20:49
Operator : JU/SJ
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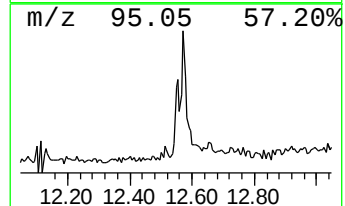
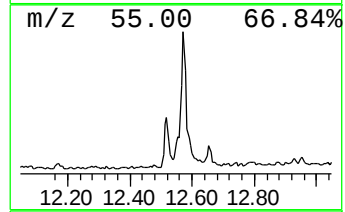
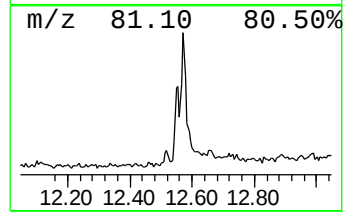
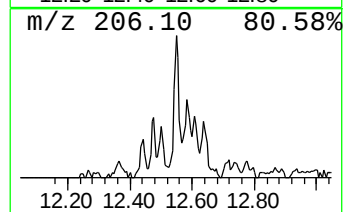
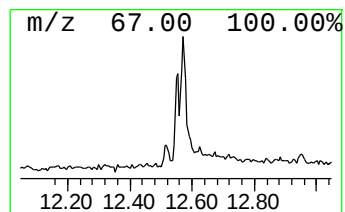
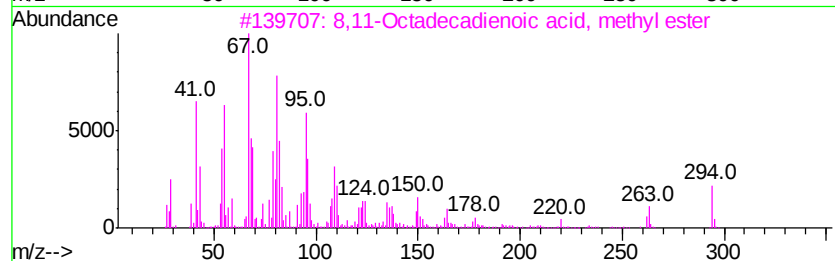
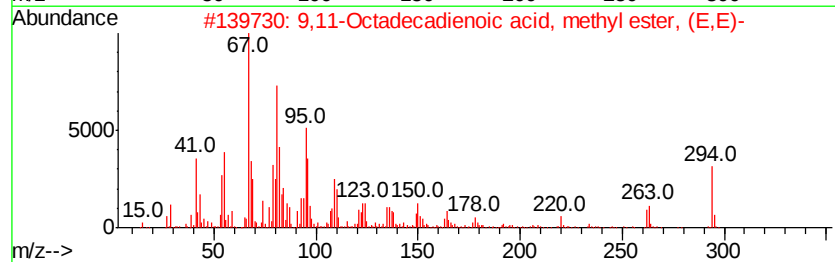
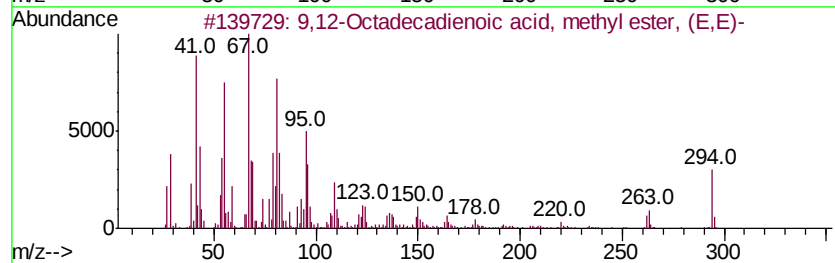
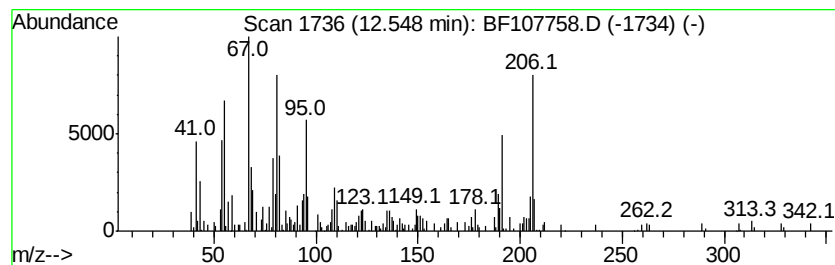
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9,12-Octadecadienoic acid, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.		
12.55	3.50 ng	191250	Phenanthrene-d10	11.49		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	70	
2	9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	64	
3	8,11-Octadecadienoic acid, methv...	294	C19H34O2	056599-58-7	64	
4	n-Propyl 9,12-octadecadienoate	322	C21H38O2	1000336-77-8	64	
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	60	



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
Data File : BF107758.D
Acq On : 27 Jul 2018 20:49
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Misc :
ALS Vial : 17 Sample Multiplier: 1

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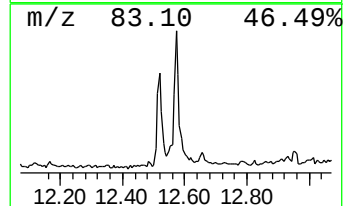
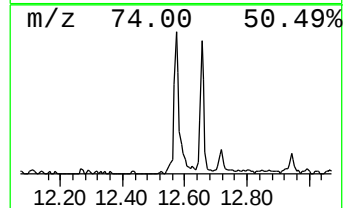
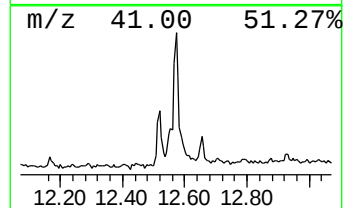
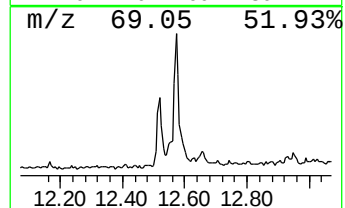
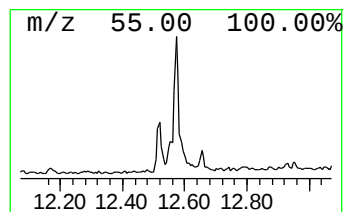
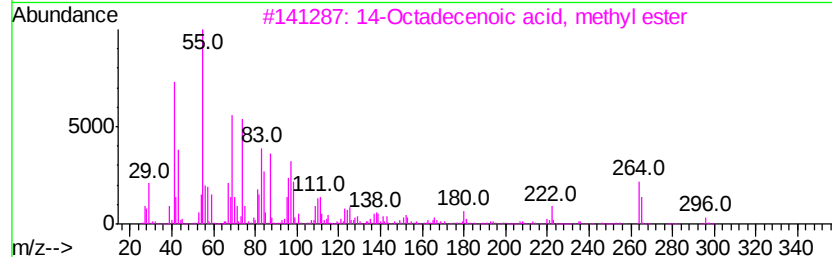
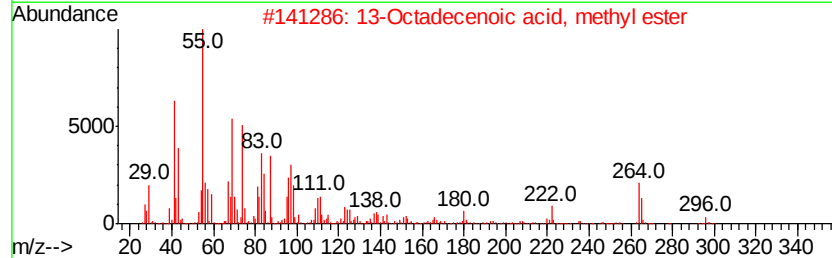
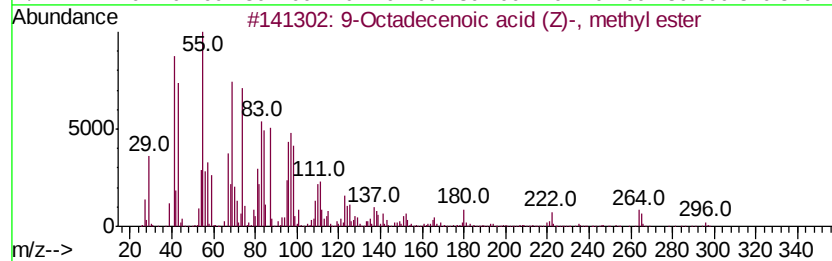
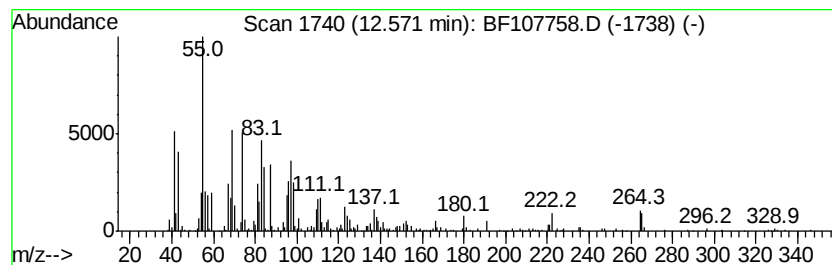
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 9-Octadecenoic acid (Z)-, m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	12.11 ng	662197	Phenanthrene-d10	11.49

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
4			15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	99
5			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
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Sample : J4121-06
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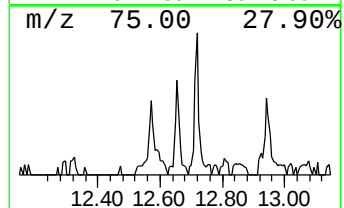
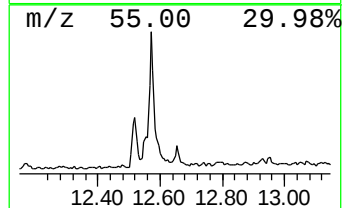
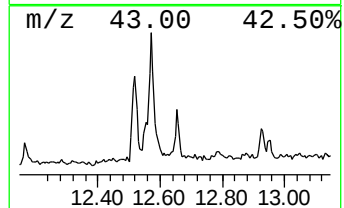
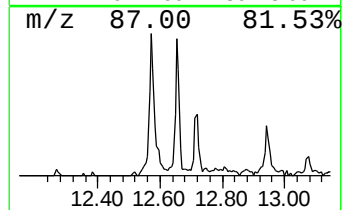
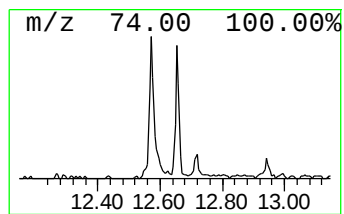
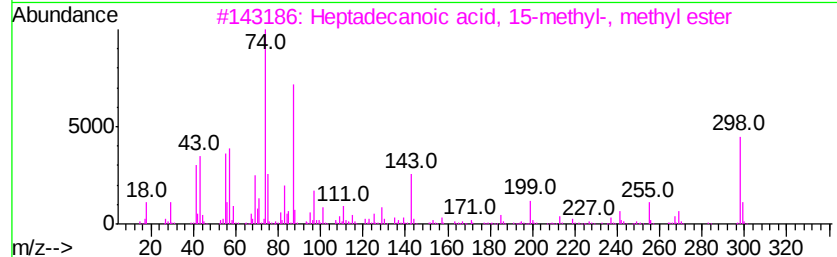
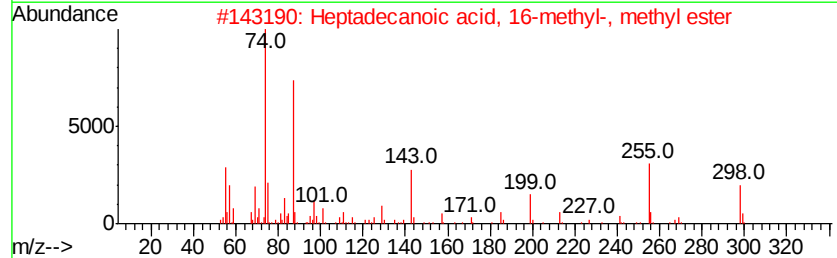
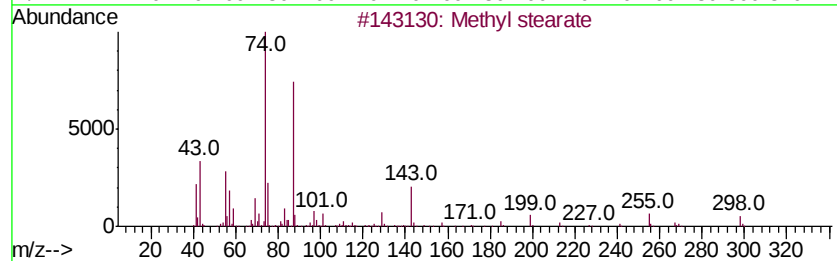
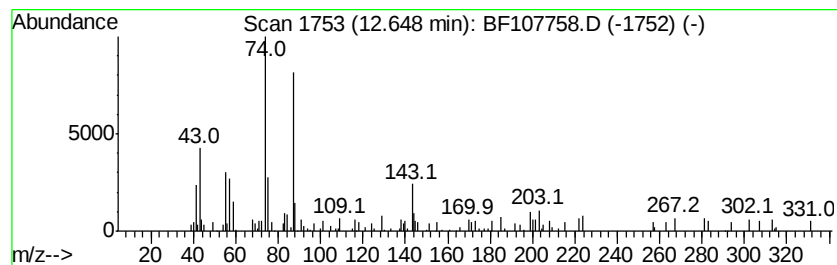
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Methyl stearate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.29 ng	125039	Phenanthrene-d10	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Methyl stearate	298 C19H38O2	000112-61-8 93
2		Heptadecanoic acid, 16-methyl-, ...	298 C19H38O2	005129-61-3 91
3		Heptadecanoic acid, 15-methyl-, ...	298 C19H38O2	054833-55-5 87
4		Dodecanoic acid, 10-methyl-, met...	228 C14H28O2	005129-65-7 83
5		Pentadecanoic acid, methyl ester	256 C16H32O2	007132-64-1 72



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
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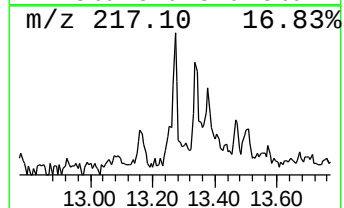
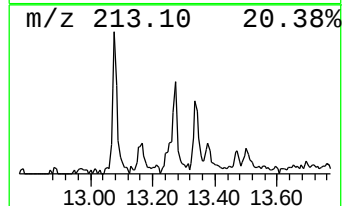
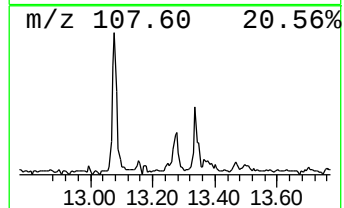
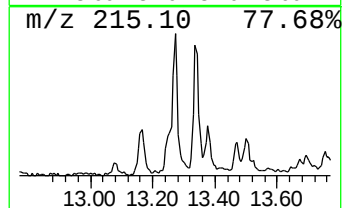
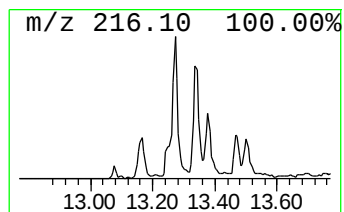
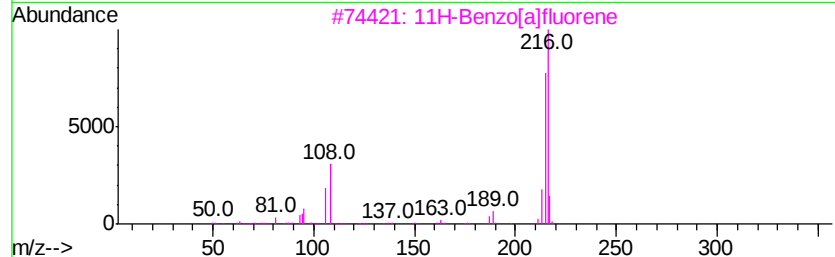
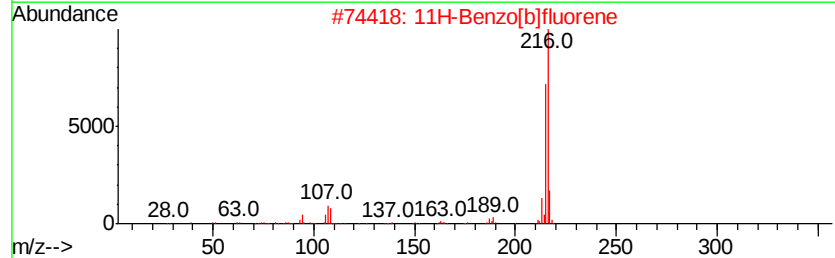
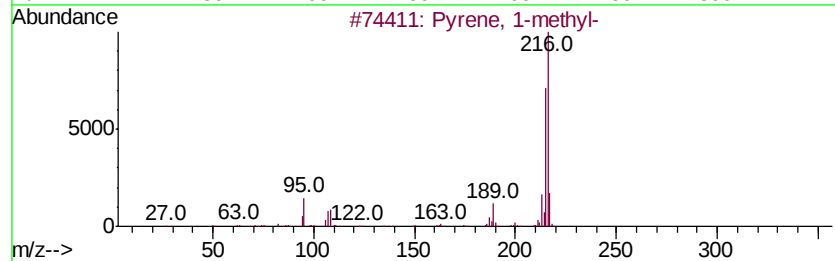
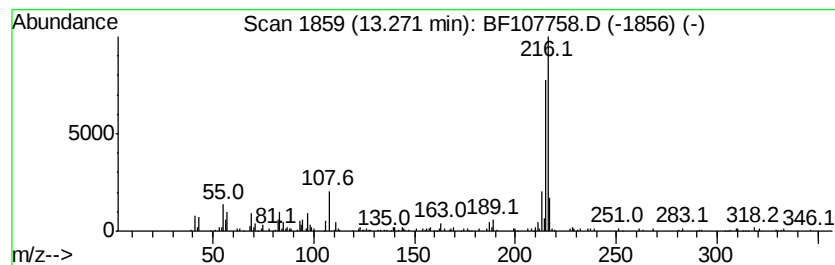
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Pyrene, 1-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.27	2.23 ng	163191	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyrene, 1-methyl-	216	C17H12	002381-21-7	87
2		11H-Benzo[b]fluorene	216	C17H12	000243-17-4	81
3		11H-Benzo[a]fluorene	216	C17H12	000238-84-6	81
4		Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	76
5		7H-Benzo[c]fluorene	216	C17H12	000205-12-9	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072718\
Data File : BF107758.D
Acq On : 27 Jul 2018 20:49
Operator : JU/SJ
Sample : J4121-06
Misc :
ALS Vial : 17 Sample Multiplier: 1

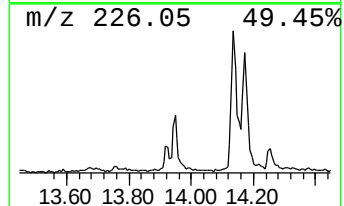
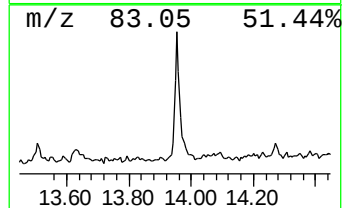
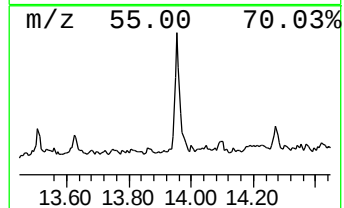
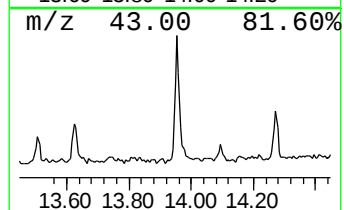
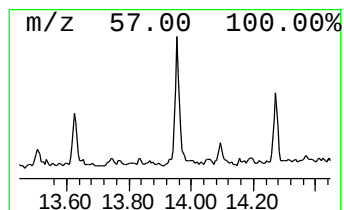
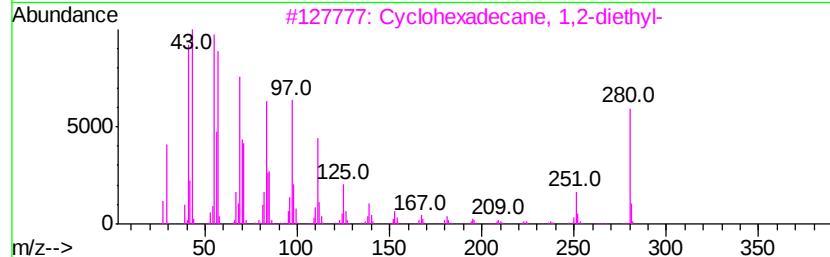
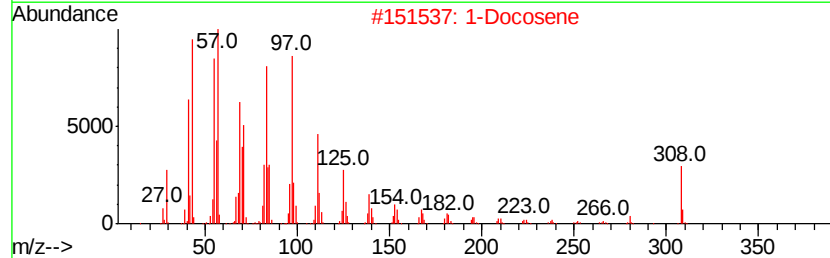
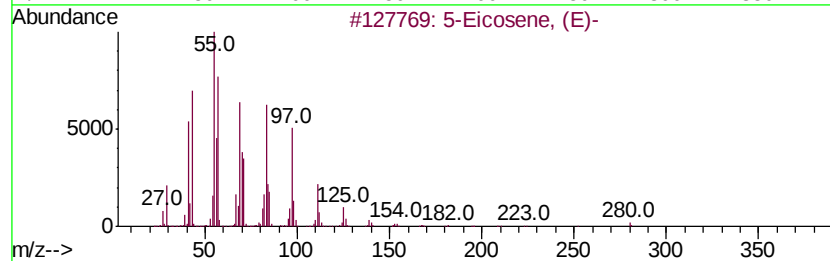
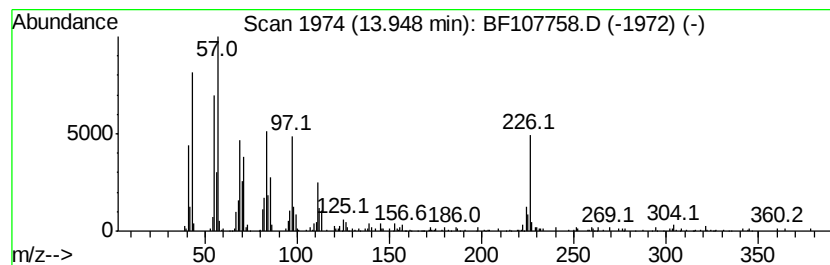
Instrument :
BNA_F
ClientSampleId :
GW-03(8-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.95	4.16 ng	304281	Chrysene-d12	14.15	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	98
2	1-Docosene	308	C22H44	001599-67-3	95
3	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	91
4	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072718\
 Data File : BF107758.D
 Acq On : 27 Jul 2018 20:49
 Operator : JU/SJ
 Sample : J4121-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GW-03(8-10)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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
2-Pentanone, 4-hy...	5.20	12.7	ng	620906	1	6.96	975483	20.0
unknown6.74	6.74	76.8	ng	3745690	1	6.96	975483	20.0
Benzene, 1-propynyl-	7.22	3.6	ng	176657	1	6.96	975483	20.0
Hexadecanoic acid...	11.86	3.9	ng	212901	4	11.49	1093950	20.0
n-Hexadecanoic acid	12.00	4.0	ng	216450	4	11.49	1093950	20.0
4H-Cyclopenta[def...	12.11	2.3	ng	125288	4	11.49	1093950	20.0
1-Nonadecene	12.52	3.3	ng	181340	4	11.49	1093950	20.0
9,12-Octadecadien...	12.55	3.5	ng	191250	4	11.49	1093950	20.0
9-Octadecenoic ac...	12.57	12.1	ng	662197	4	11.49	1093950	20.0
Methyl stearate	12.65	2.3	ng	125039	4	11.49	1093950	20.0
Pyrene, 1-methyl-	13.27	2.2	ng	163191	5	14.15	1462700	20.0
5-Eicosene, (E)-	13.95	4.2	ng	304281	5	14.15	1462700	20.0