

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083118\
 Data File : BF108694.D
 Acq On : 31 Aug 2018 17:35
 Operator : JU/SJ
 Sample : J4720-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BZTRANS-3

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-BF083018.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	5.237	489	493	500	rBV	23435	32872	2.42%	0.195%
2	5.643	558	562	580	rBV	159423	598597	44.13%	3.558%
3	6.643	728	732	751	rBV	264284	888070	65.47%	5.279%
4	6.772	751	754	786	rVV	614129	1356390	100.00%	8.062%
5	7.001	789	793	813	rVV	189038	470522	34.69%	2.797%
6	7.154	815	819	842	rVV	580464	880533	64.92%	5.234%
7	7.566	886	889	916	rBV	235596	709786	52.33%	4.219%
8	8.284	1007	1011	1036	rBV	299409	560843	41.35%	3.334%
9	9.354	1189	1193	1223	rBV	920383	1298878	95.76%	7.720%
10	9.742	1256	1259	1273	rBV	274289	335682	24.75%	1.995%
11	10.042	1306	1310	1327	rBV	440895	564310	41.60%	3.354%
12	10.442	1376	1378	1382	rVB	15970	14956	1.10%	0.089%
13	10.836	1442	1445	1457	rBV	424086	678210	50.00%	4.031%
14	10.913	1457	1458	1463	rVB4	16753	22677	1.67%	0.135%
15	11.366	1529	1535	1538	rBV4	24212	40017	2.95%	0.238%
16	11.460	1545	1551	1555	rBV4	17472	38410	2.83%	0.228%
17	11.542	1561	1565	1567	rBV	411024	503071	37.09%	2.990%
18	11.566	1567	1569	1577	rVB	331699	402132	29.65%	2.390%
19	11.795	1604	1608	1619	rBV3	18619	38953	2.87%	0.232%
20	12.007	1641	1644	1647	rBV4	10556	16814	1.24%	0.100%
21	12.042	1647	1650	1653	rVV2	85450	97733	7.21%	0.581%
22	12.072	1653	1655	1659	rVB	28704	36024	2.66%	0.214%
23	12.154	1666	1669	1672	rBV2	26636	34734	2.56%	0.206%
24	12.342	1698	1701	1703	rBV2	16367	19700	1.45%	0.117%
25	12.372	1703	1706	1718	rVB2	52890	90752	6.69%	0.539%
26	12.589	1741	1743	1746	rVB3	20395	18490	1.36%	0.110%
27	12.760	1768	1772	1783	rBV	427375	569606	41.99%	3.386%
28	12.913	1796	1798	1801	rBV2	17514	16624	1.23%	0.099%
29	12.989	1808	1811	1829	rVB	298684	466987	34.43%	2.776%
30	13.119	1829	1833	1843	rBV	1160163	1260900	92.96%	7.495%
31	13.319	1865	1867	1871	rBV3	39985	38933	2.87%	0.231%
32	13.548	1904	1906	1909	rBV	36274	34902	2.57%	0.207%
33	13.995	1979	1982	1983	rBV2	61359	49269	3.63%	0.293%
34	14.019	1984	1986	1990	rBV3	64802	97678	7.20%	0.581%

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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	14.130	2003	2005	2009	rBV	104325	95698	7.06%	0.569%
36	14.195	2011	2016	2019	rBV2	561640	739738	54.54%	4.397%
37	14.613	2085	2087	2092	rVB	130954	138533	10.21%	0.823%
38	14.660	2093	2095	2101	rVB4	92137	129301	9.53%	0.769%
39	14.871	2128	2131	2139	rBV3	69819	132120	9.74%	0.785%
40	15.101	2167	2170	2177	rVB2	185921	218606	16.12%	1.299%
41	15.301	2198	2204	2211	rVB2	538609	815100	60.09%	4.845%
42	15.371	2213	2216	2233	rVB9	103454	264967	19.53%	1.575%
43	15.707	2267	2273	2277	rBV3	92050	199177	14.68%	1.184%
44	15.754	2277	2281	2295	rVB	234839	463079	34.14%	2.752%
45	15.930	2308	2311	2321	rVB	225948	368131	27.14%	2.188%
46	16.177	2348	2353	2362	rVB	321373	524545	38.67%	3.118%
47	17.048	2498	2501	2510	rVB2	117439	217394	16.03%	1.292%
48	17.371	2553	2556	2567	rVB4	107333	233504	17.22%	1.388%

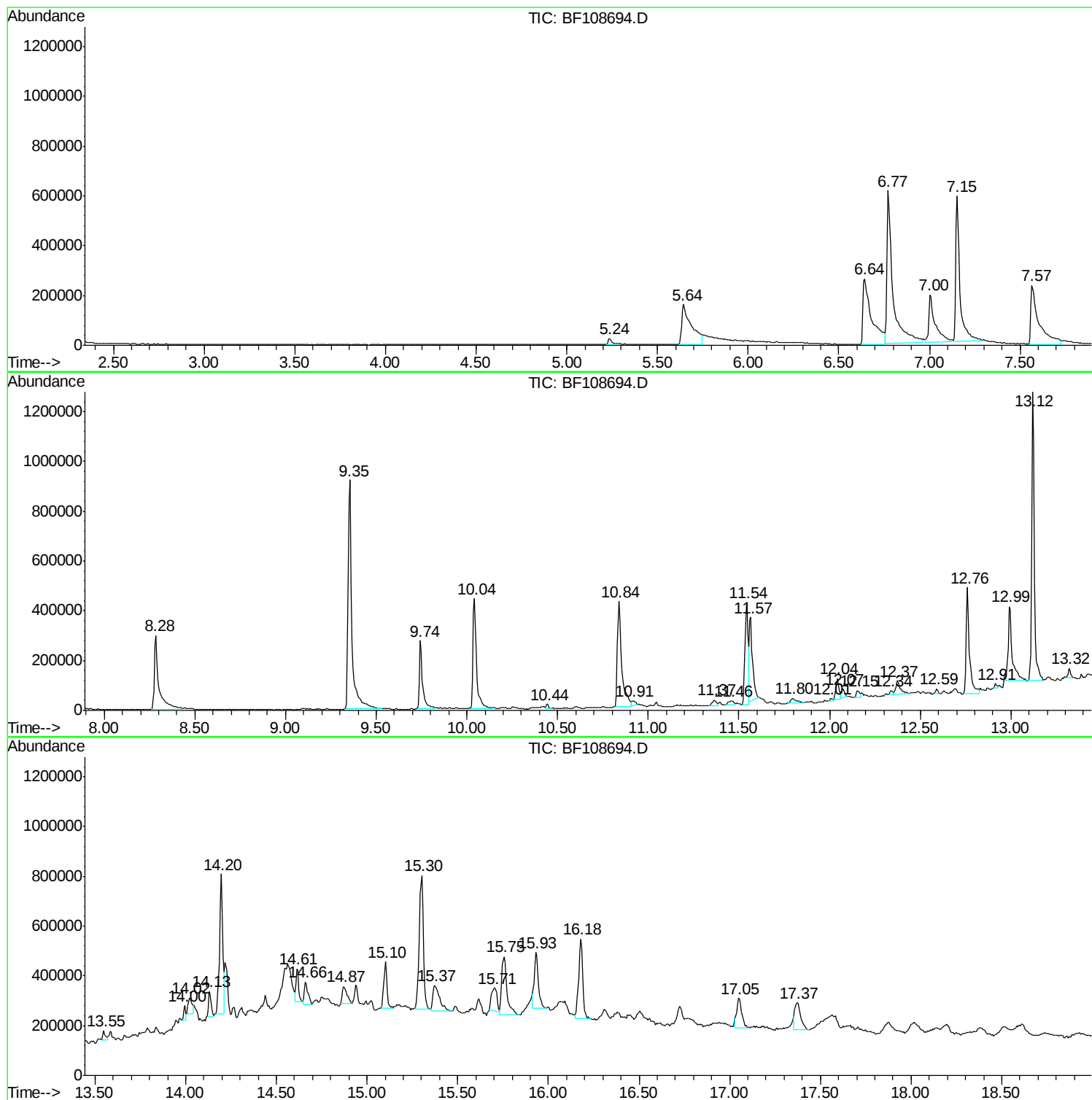
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF083018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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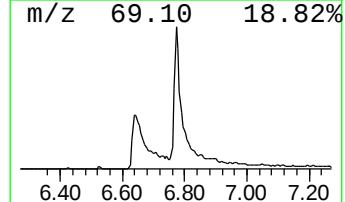
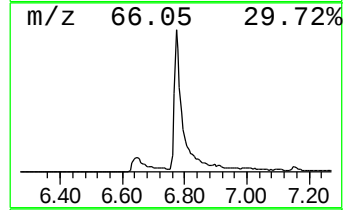
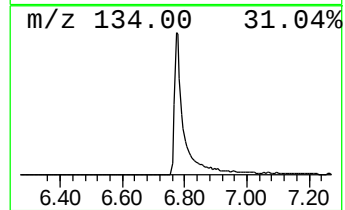
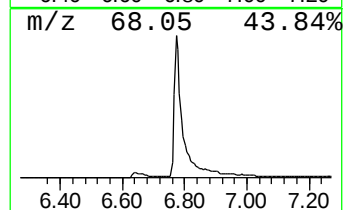
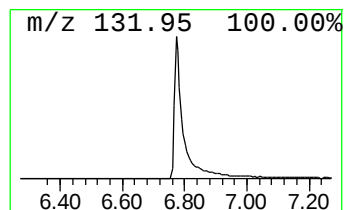
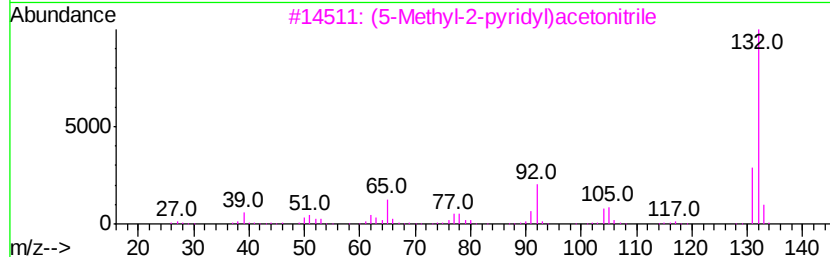
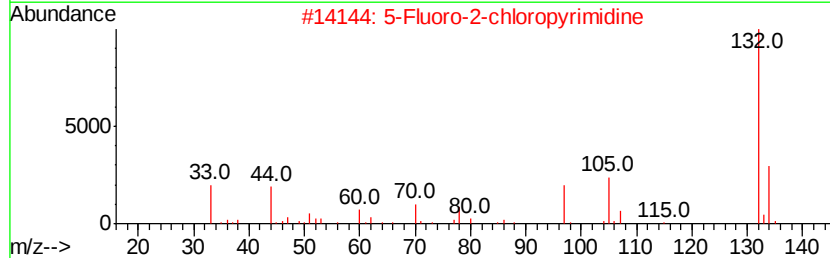
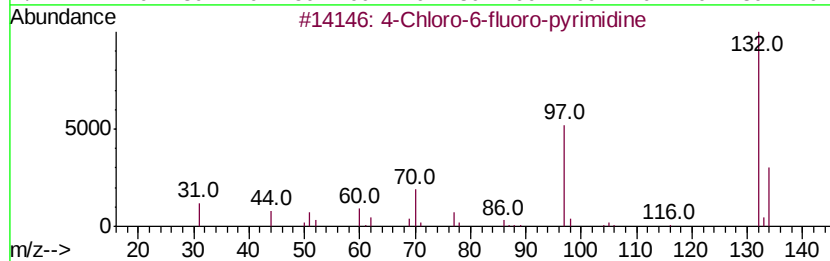
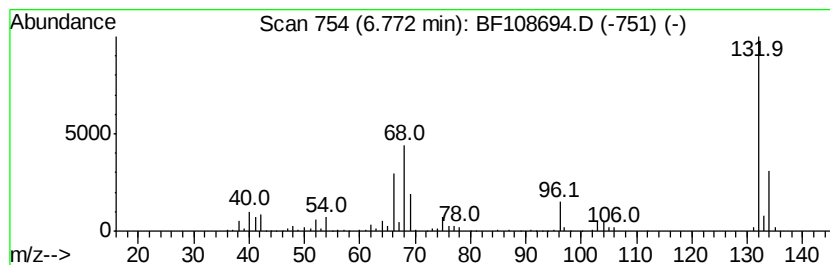
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	57.65 ng	1356390	1,4-Dichlorobenzene-d4	7.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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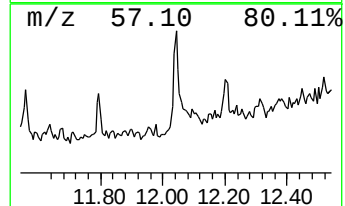
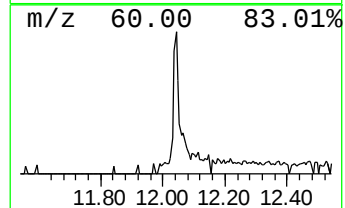
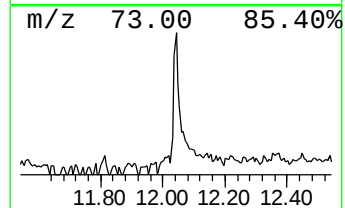
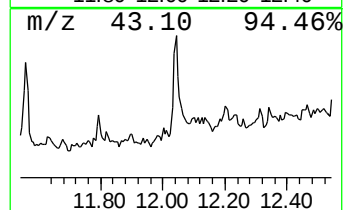
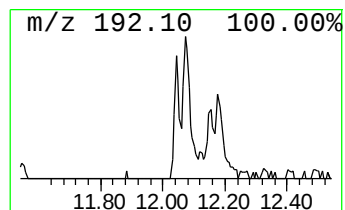
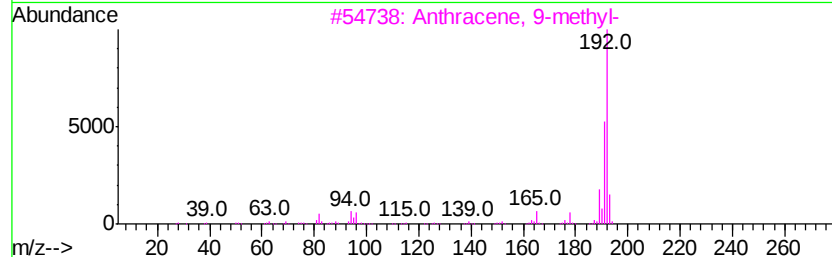
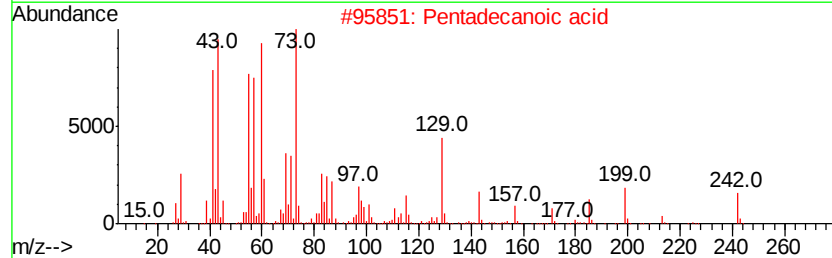
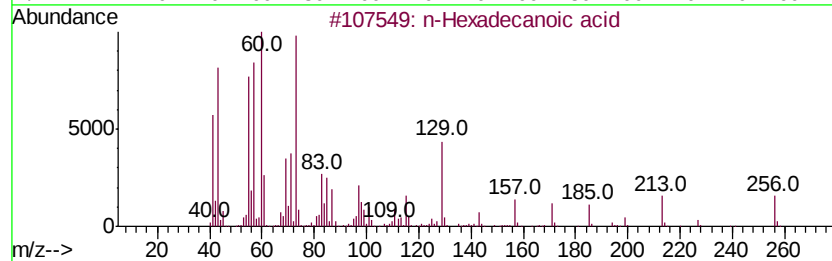
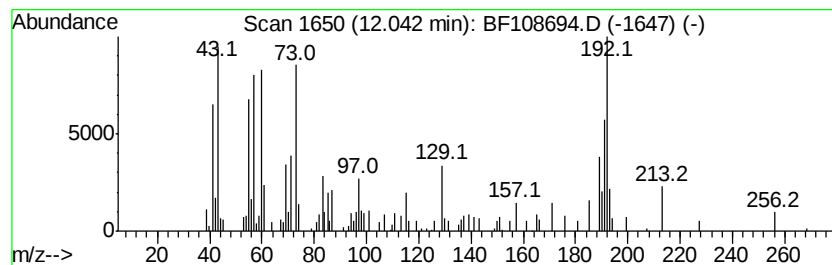
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	3.89 ng	97733	Phenanthrene-d10	11.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	30
3	Anthracene, 9-methyl-	192	C15H12	000779-02-2	30
4	Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	27
5	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	27



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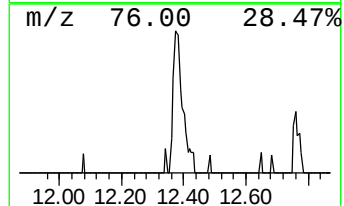
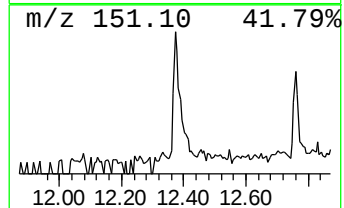
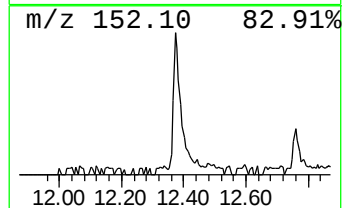
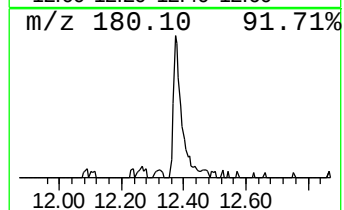
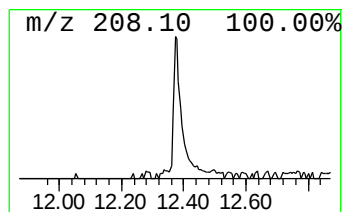
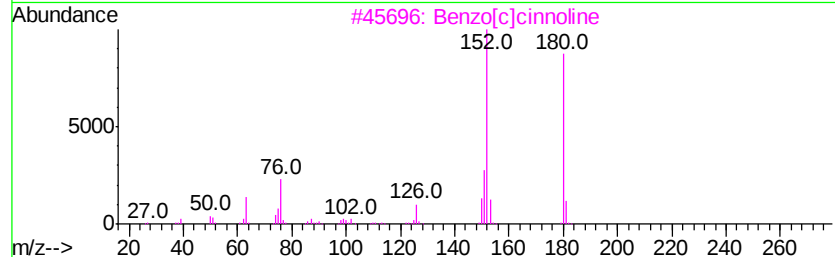
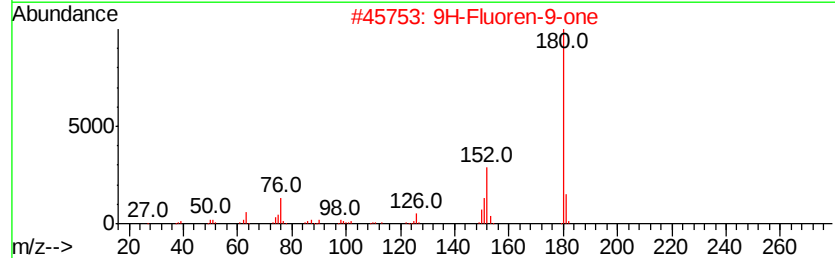
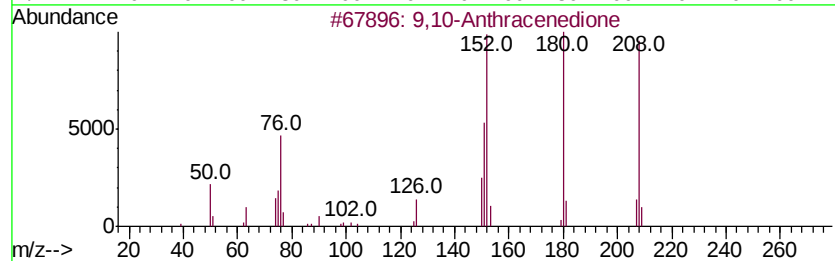
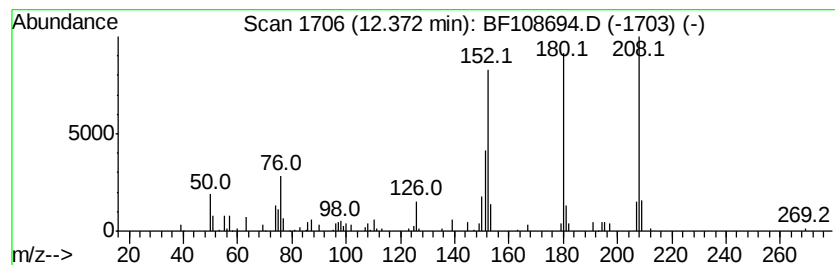
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 9,10-Anthracenedione Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.37	3.61 ng	90752	Phenanthrene-d10	11.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,10-Anthracenedione	208	C14H8O2	000084-65-1	98
2			9H-Fluoren-9-one	180	C13H8O	000486-25-9	70
3			Benzo[c]cinnoline	180	C12H8N2	000230-17-1	62
4			1H-Phenalen-1-one	180	C13H8O	000548-39-0	60
5			Benzo[h]cinnoline	180	C12H8N2	000230-31-9	60



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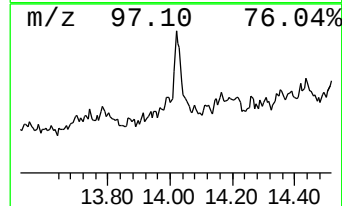
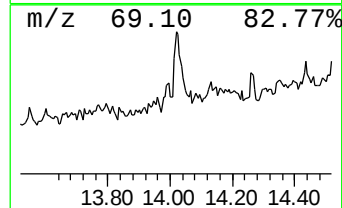
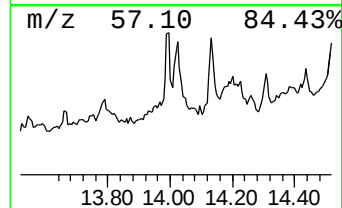
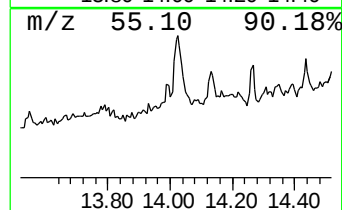
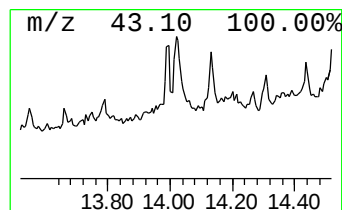
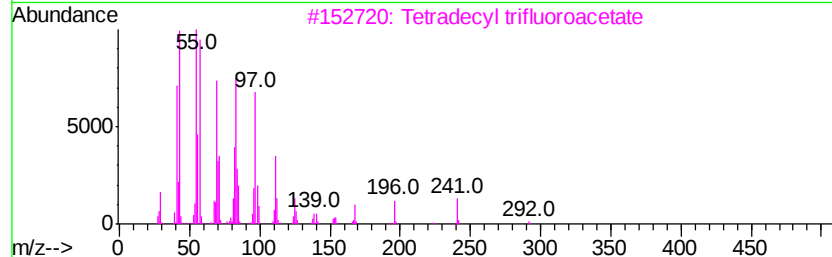
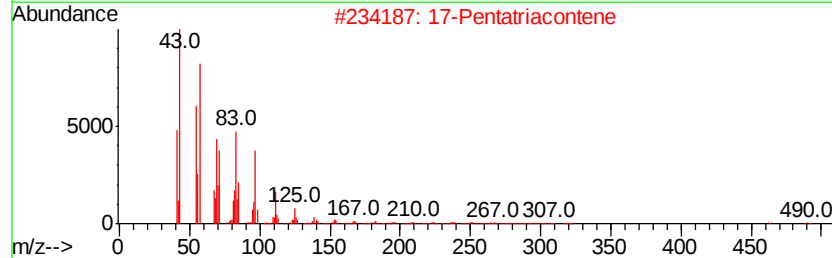
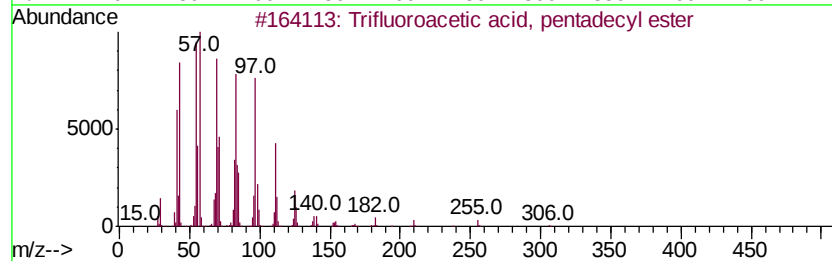
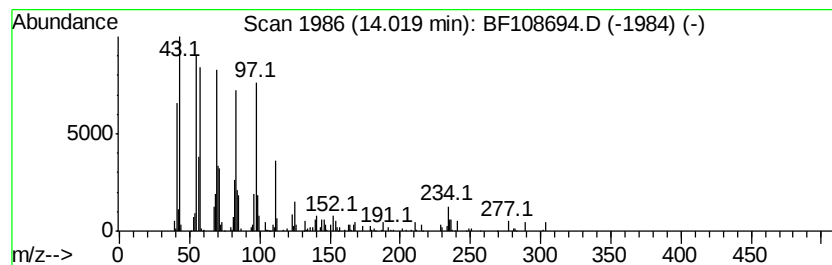
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.02	2.64 ng	97678	Chrysene-d12	14.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
2		17-Pentatriacontene	491	C35H70	006971-40-0	87
3		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	83
4		E-15-Heptadecenal	252	C17H32O	1000130-97-9	58
5		1-Pentadecene	210	C15H30	013360-61-7	58



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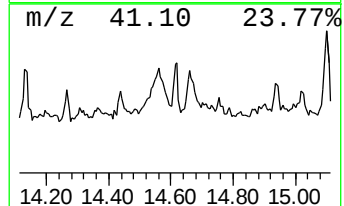
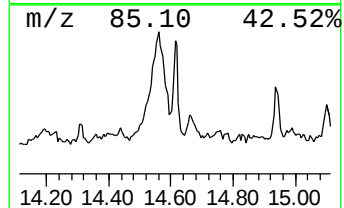
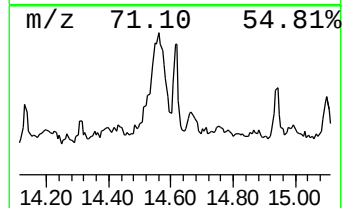
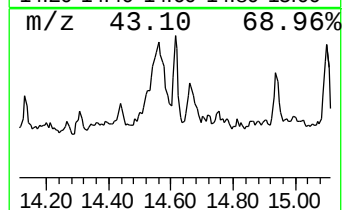
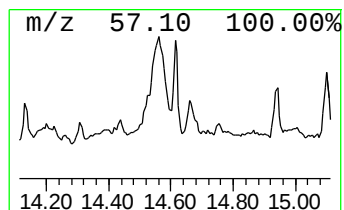
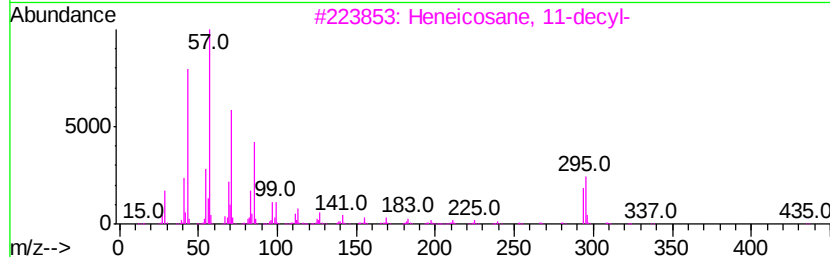
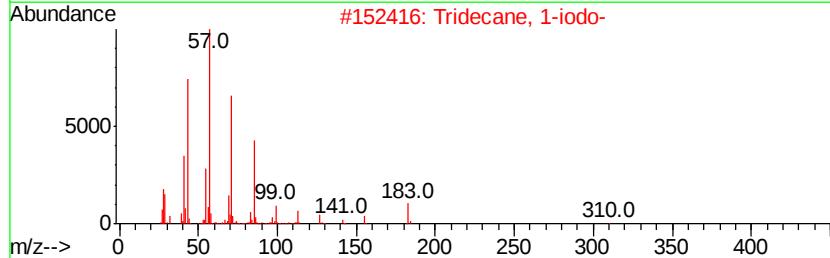
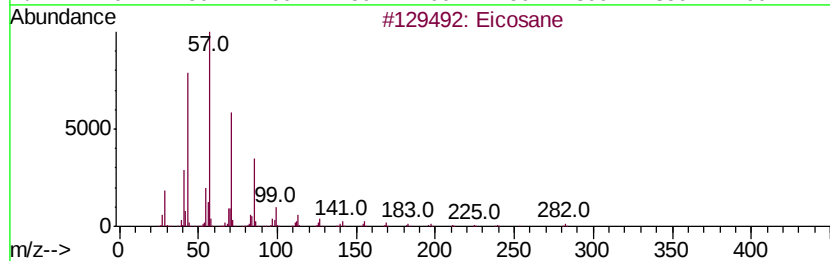
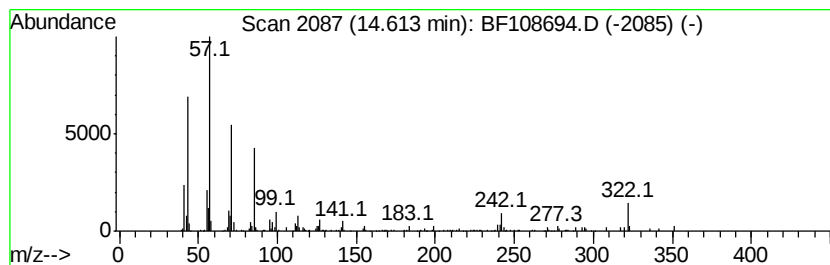
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
14.61	3.75 ng	138533	Chrysene-d12		14.20
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	68
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	68
3	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	64
4	Nonadecane	268	C19H40	000629-92-5	64
5	Octadecane	254	C18H38	000593-45-3	59



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108694.D
Acq On : 31 Aug 2018 17:35
Operator : JU/SJ
Sample : J4720-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

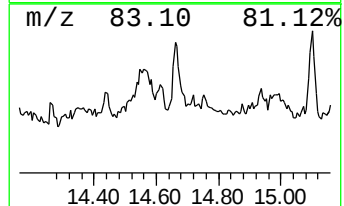
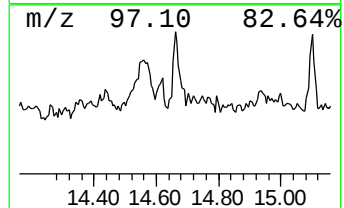
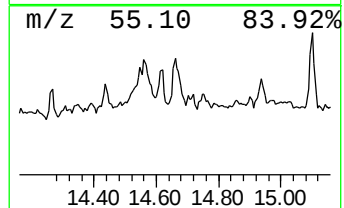
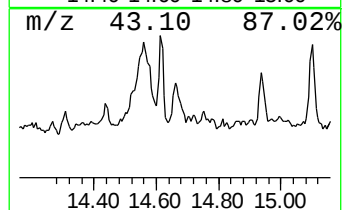
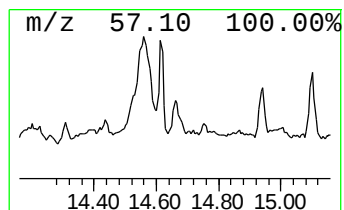
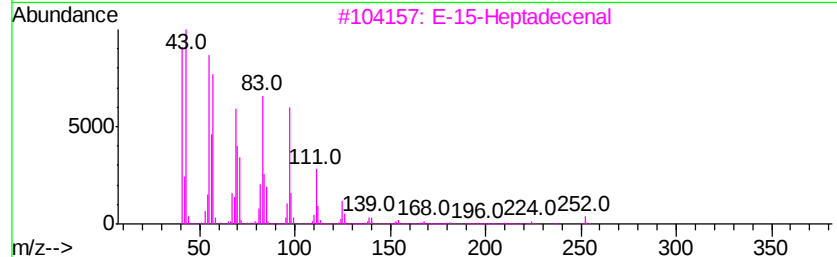
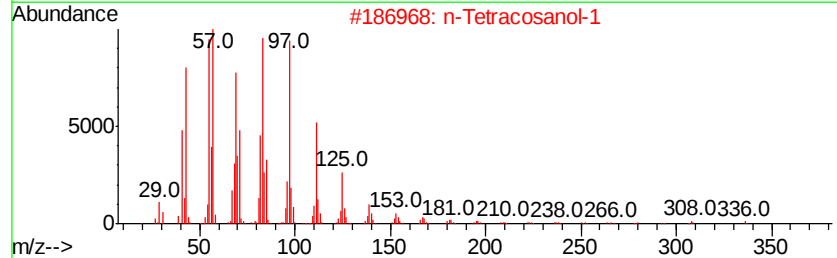
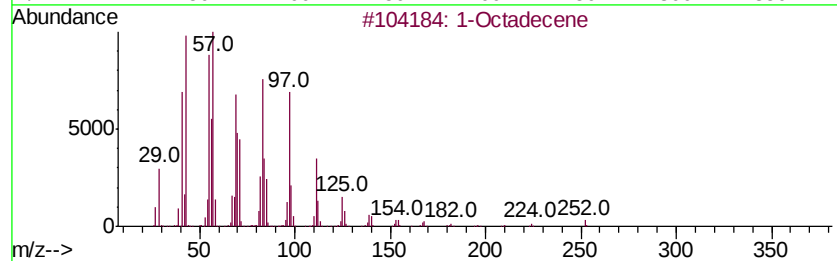
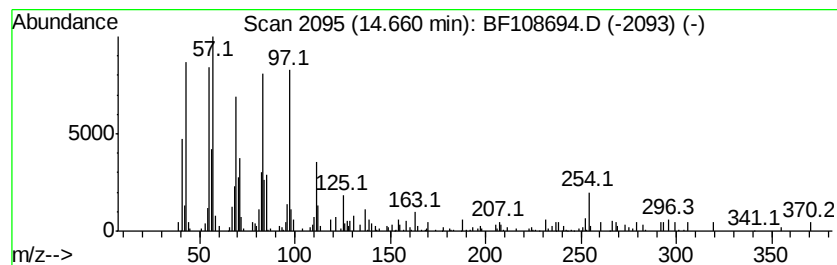
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Octadecene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.66	3.50 ng	129301	Chrysene-d12	14.20
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octadecene	252 C18H36	000112-88-9	91
2	n-Tetracosanol-1	354 C24H50O	000506-51-4	87
3	E-15-Heptadecenal	252 C17H32O	1000130-97-9	86
4	8-Heptadecene	238 C17H34	002579-04-6	83
5	Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3	83



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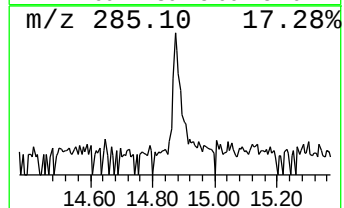
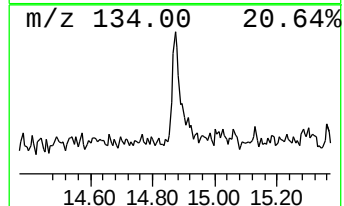
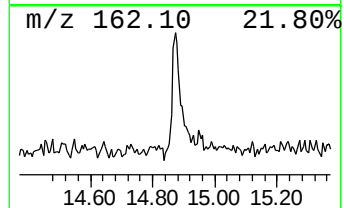
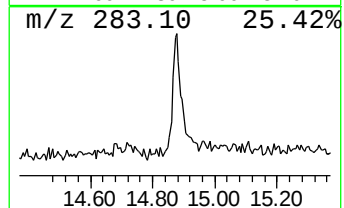
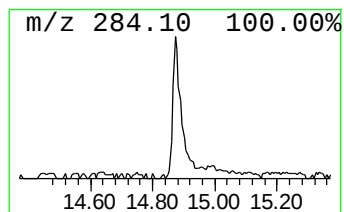
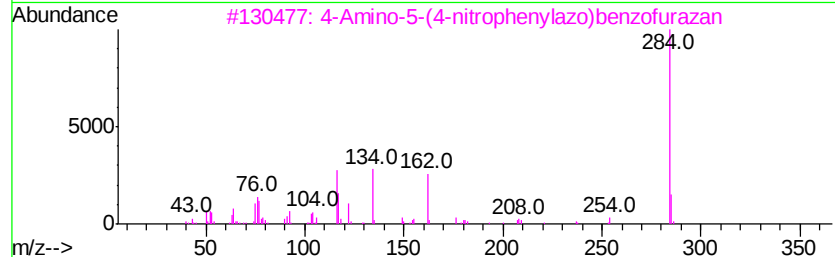
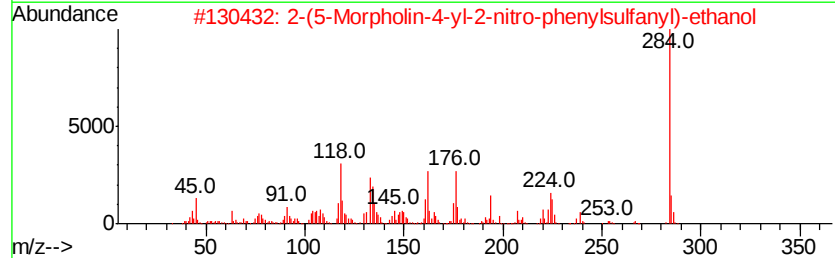
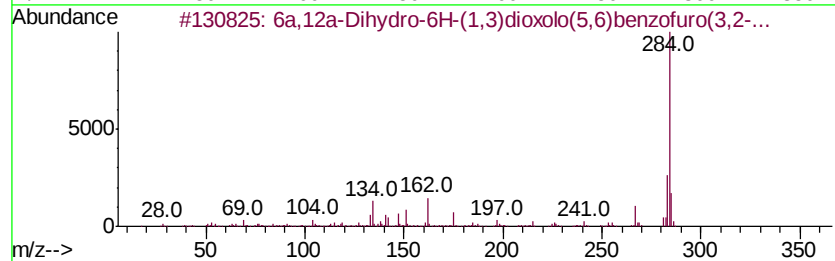
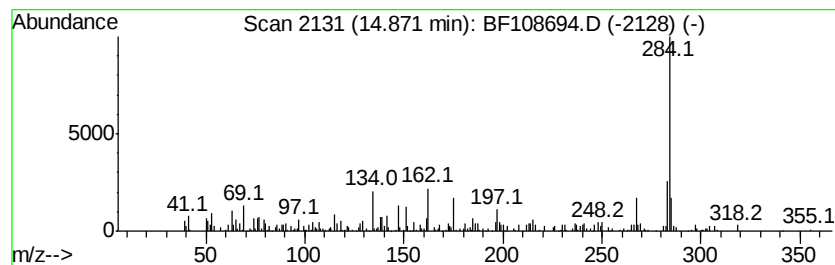
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 6a,12a-Dihydro-6H-(1,3)diox... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.87	3.57 ng	132120	Chrysene-d12	14.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6a,12a-Dihydro-6H-(1,3)dioxolo(5...	284	C16H12O5	022091-18-5	91
2	2-(5-Morpholin-4-yl-2-nitro-phen...	284	C12H16N2O4S	1000294-41-6	53
3	4-Amino-5-(4-nitrophenylazo)benz...	284	C12H8N6O3	166766-07-0	53
4	9,10-Anthraquinone diimine, N,N'...	284	C18H12N4	1000142-29-9	49
5	6H-Benzofuro[3,2-c][1]benzopyran...	284	C17H16O4	000606-91-7	49



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
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Misc :
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Instrument :
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ClientSampleId :
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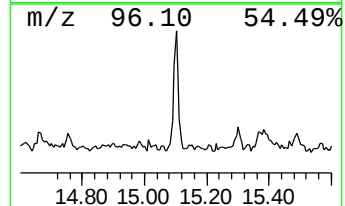
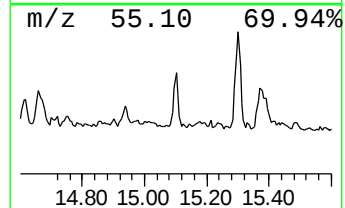
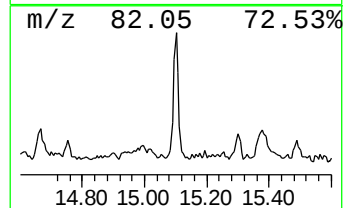
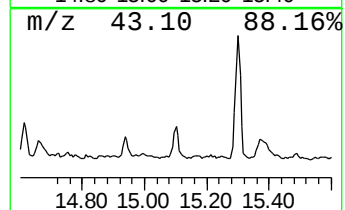
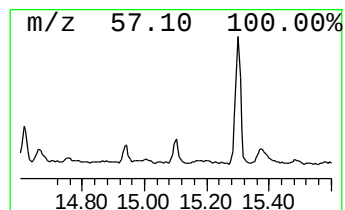
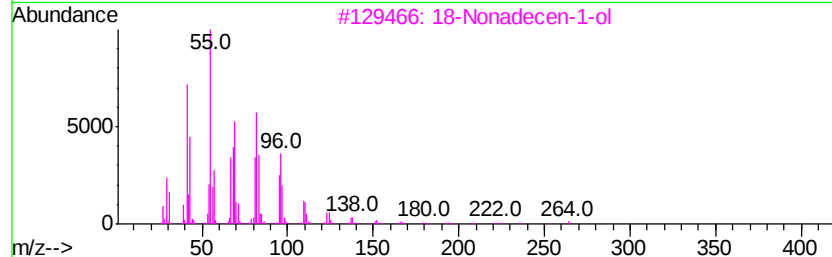
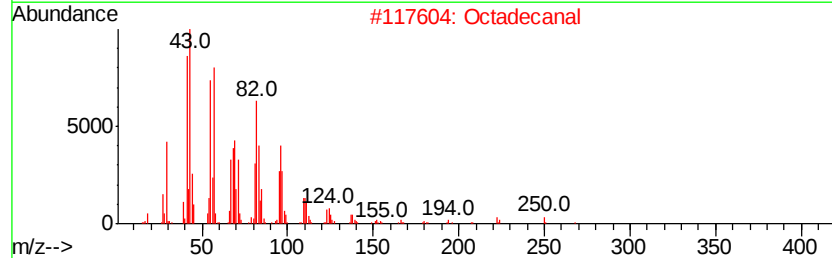
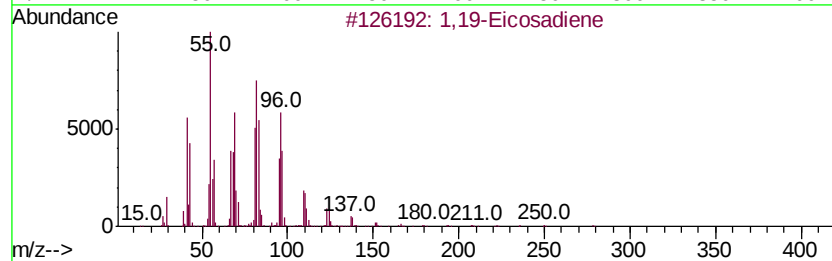
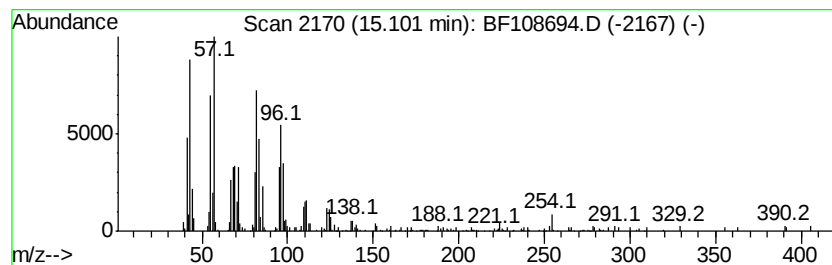
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,19-Eicosadiene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	9.44 ng	218606	Perylene-d12	15.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene		278	C20H38	014811-95-1	87
2	Octadecanal		268	C18H36O	000638-66-4	86
3	18-Nonadecen-1-ol		282	C19H38O	1000142-89-2	80
4	(E)-Dodec-2-enyl isobutyl carbonate		284	C17H32O3	1000372-78-7	78
5	1,16-Hexadecanediol		258	C16H34O2	007735-42-4	74



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
Data File : BF108694.D
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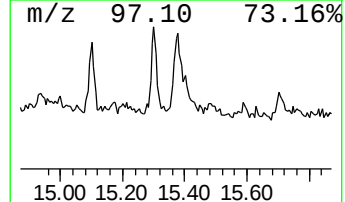
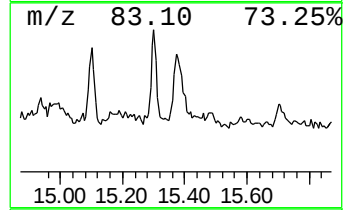
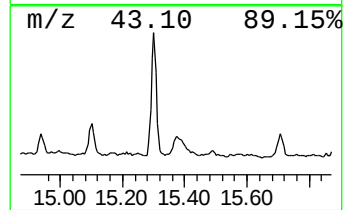
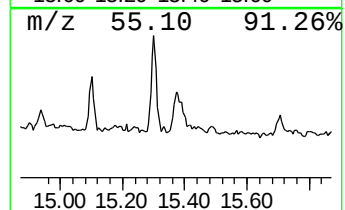
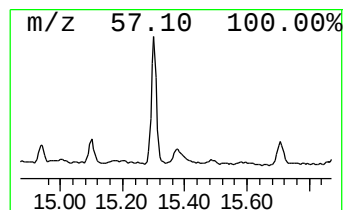
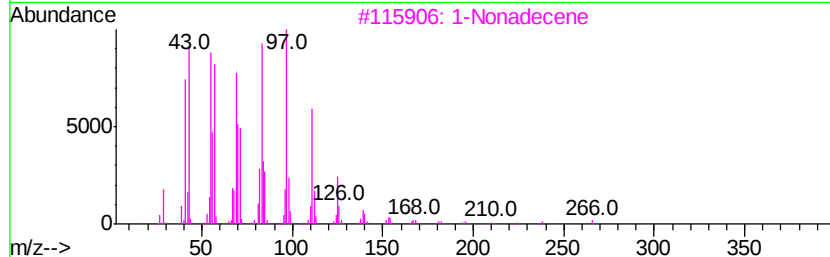
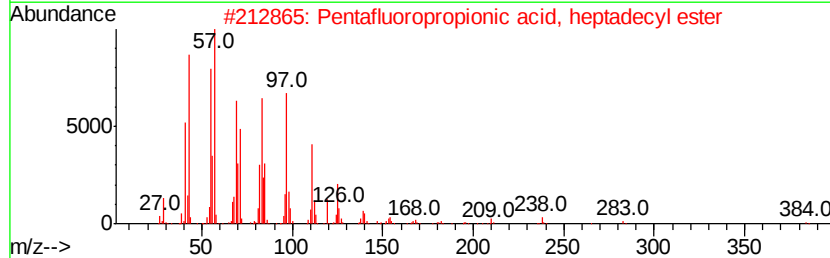
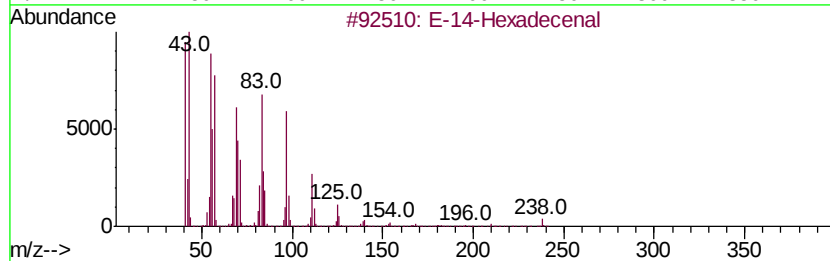
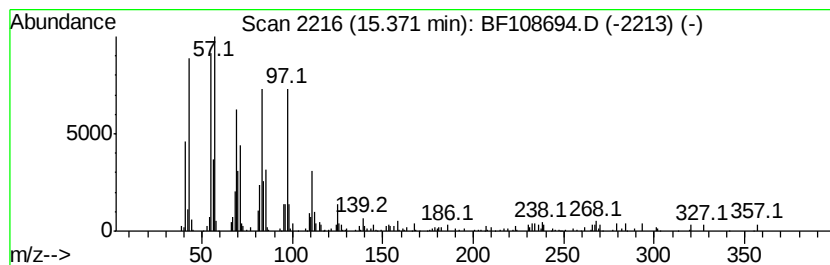
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 E-14-Hexadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	11.44 ng	264967	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-14-Hexadecenal	238	C16H30O	330207-53-9	93
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	93
3		1-Nonadecene	266	C19H38	018435-45-5	92
4		1-Docosene	308	C22H44	001599-67-3	90
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
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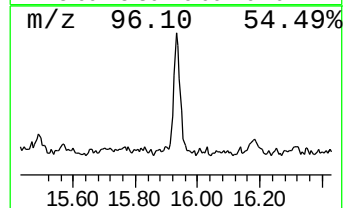
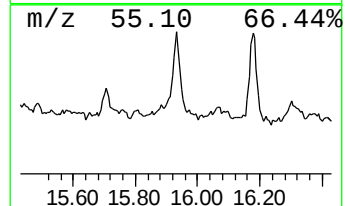
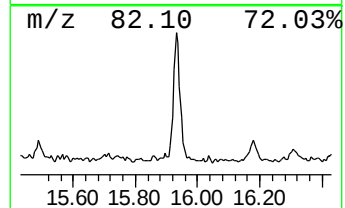
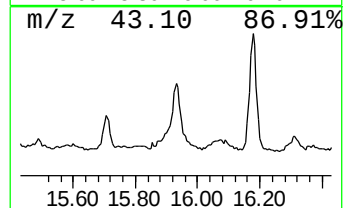
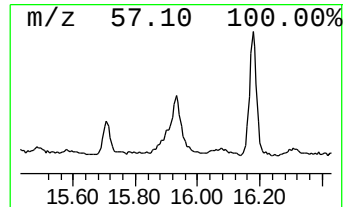
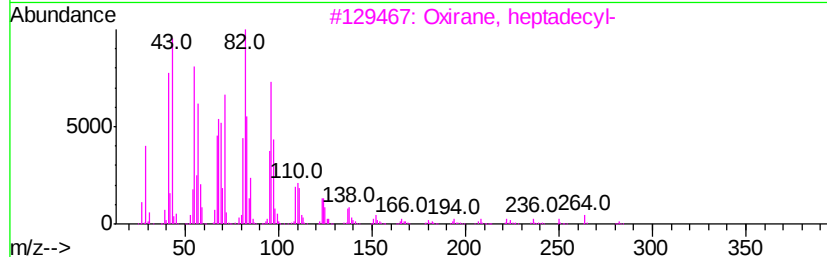
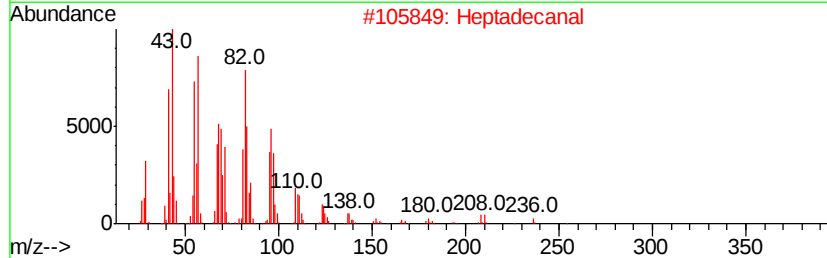
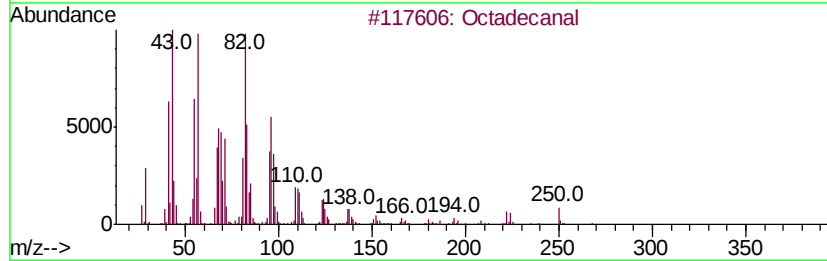
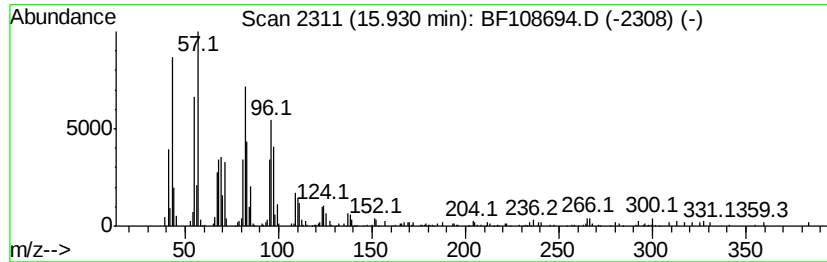
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.93	15.90 ng	368131	Perylene-d12	15.75		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanal	268	C18H36O	000638-66-4	94
2		Heptadecanal	254	C17H34O	1000376-70-0	93
3		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	86
4		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83
5		1,13-Tetradecadiene	194	C14H26	021964-49-8	78



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF083118\
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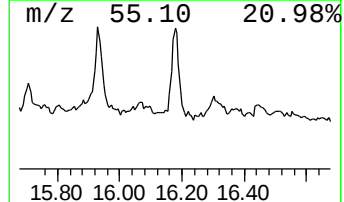
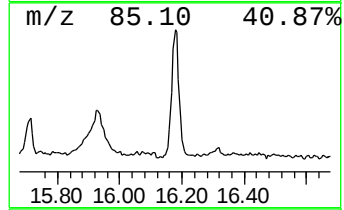
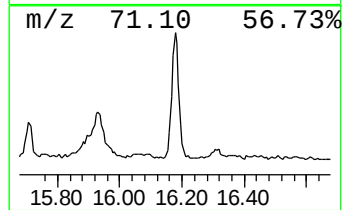
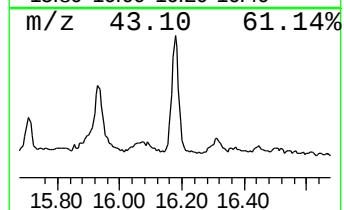
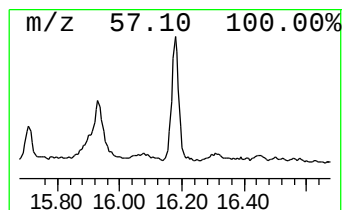
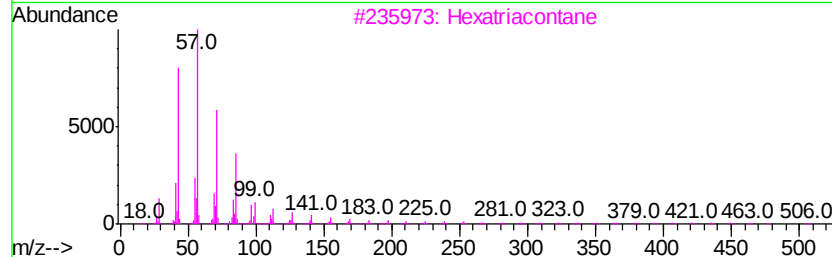
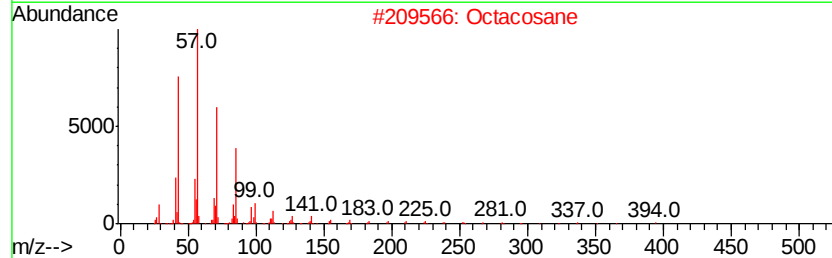
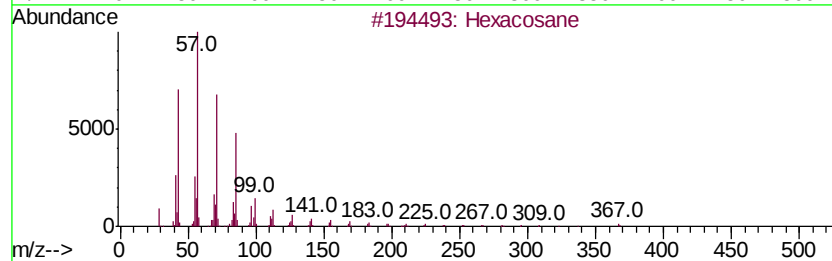
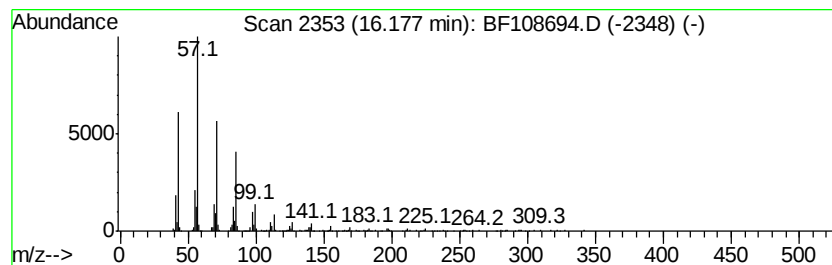
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Hexacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	22.65 ng	524545	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	94
2		Octacosane	394	C28H58	000630-02-4	91
3		Hexatriacontane	507	C36H74	000630-06-8	91
4		Pentacosane	352	C25H52	000629-99-2	91
5		Heptacosane	380	C27H56	000593-49-7	91



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Misc :
ALS Vial : 9 Sample Multiplier: 1

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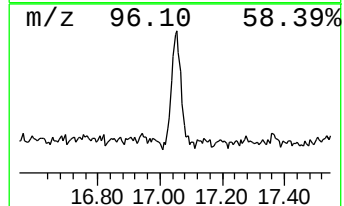
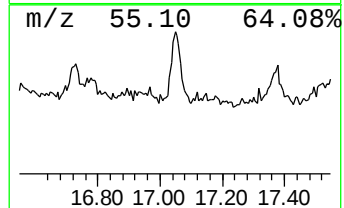
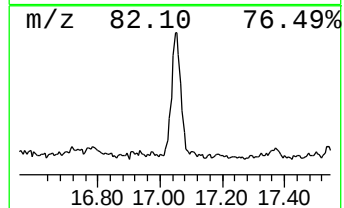
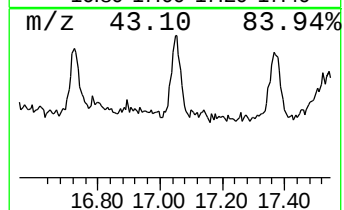
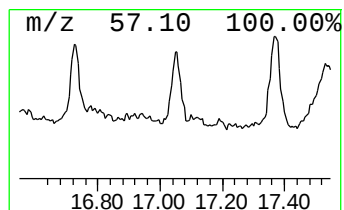
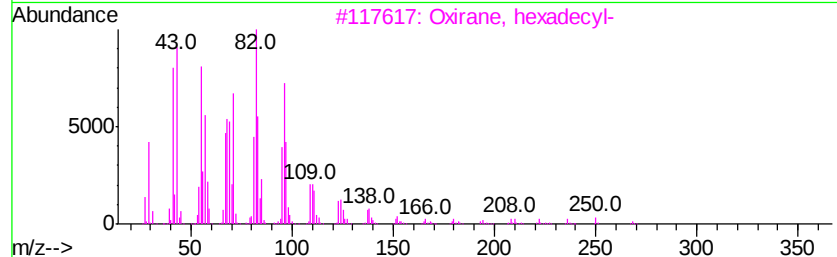
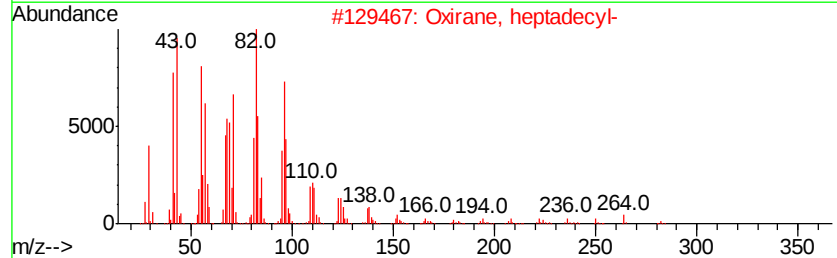
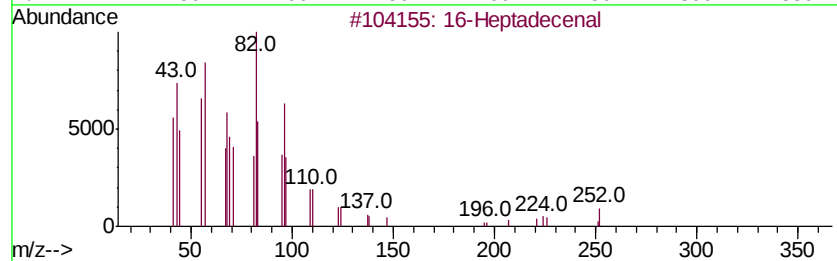
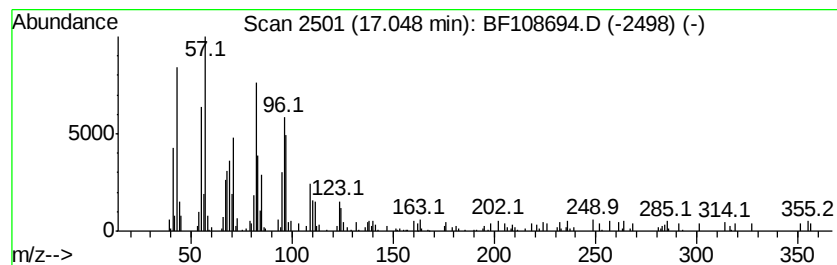
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 16-Heptadecenal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.05	9.39 ng	217394	Perylene-d12	15.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	16-Heptadecenal	252	C17H32O	1000144-57-9	95
2		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	90
3		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	74
4		Octadecanal	268	C18H36O	000638-66-4	58
5		1,16-Hexadecanediol	258	C16H34O2	007735-42-4	52



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF083118\
Data File : BF108694.D
Acq On : 31 Aug 2018 17:35
Operator : JU/SJ
Sample : J4720-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
BZTRANS-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF083018.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
unknown6.77	6.77	57.6	ng	1356390	1	7.00	470522	20.0
n-Hexadecanoic acid	12.04	3.9	ng	97733	4	11.54	503071	20.0
9,10-Anthracenedione	12.37	3.6	ng	90752	4	11.54	503071	20.0
Trifluoroacetic a...	14.02	2.6	ng	97678	5	14.20	739738	20.0
Eicosane	14.61	3.8	ng	138533	5	14.20	739738	20.0
1-Octadecene	14.66	3.5	ng	129301	5	14.20	739738	20.0
6a,12a-Dihydro-6H...	14.87	3.6	ng	132120	5	14.20	739738	20.0
1,19-Eicosadiene	15.10	9.4	ng	218606	6	15.75	463079	20.0
E-14-Hexadecenal	15.37	11.4	ng	264967	6	15.75	463079	20.0
Octadecanal	15.93	15.9	ng	368131	6	15.75	463079	20.0
Hexacosane	16.18	22.6	ng	524545	6	15.75	463079	20.0
16-Heptadecenal	17.05	9.4	ng	217394	6	15.75	463079	20.0