

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
 Data File : BF109094.D
 Acq On : 18 Sep 2018 14:39
 Operator : JU/SJ
 Sample : J4940-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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	4.919	434	439	446	rVB	84077	107470	3.12%	0.323%
2	5.331	504	509	512	rBV	2904757	2923352	84.74%	8.798%
3	6.360	678	684	687	rBV	2904120	3083228	89.38%	9.279%
4	6.489	701	706	709	rBV	3355822	3061341	88.74%	9.213%
5	6.719	741	745	749	rBV	1135651	880200	25.51%	2.649%
6	6.878	768	772	775	rBV	2834912	2389727	69.27%	7.192%
7	7.278	835	840	843	rBV	2069556	1967932	57.05%	5.923%
8	8.001	959	963	966	rBV	1364931	1101951	31.94%	3.316%
9	9.077	1141	1146	1149	rBV	3956448	3449744	100.00%	10.382%
10	9.466	1209	1212	1216	rBV	284522	252277	7.31%	0.759%
11	9.748	1256	1260	1264	rBV2	1447025	1250889	36.26%	3.765%
12	10.530	1389	1393	1397	rBV	1769697	1750244	50.74%	5.268%
13	11.224	1508	1511	1514	rBV	1363812	1221266	35.40%	3.676%
14	11.248	1514	1515	1518	rVB	83279	49068	1.42%	0.148%
15	11.760	1598	1602	1612	rBV3	96137	170419	4.94%	0.513%
16	12.430	1710	1716	1720	rBV	200009	182314	5.28%	0.549%
17	12.548	1731	1736	1748	rBV2	169943	277514	8.04%	0.835%
18	12.654	1749	1754	1758	rVB2	131584	157690	4.57%	0.475%
19	12.807	1776	1780	1784	rBV	2961687	2800081	81.17%	8.427%
20	12.989	1808	1811	1814	rVB	36245	38294	1.11%	0.115%
21	13.054	1818	1822	1825	rVB2	40248	46147	1.34%	0.139%
22	13.724	1932	1936	1945	rVB2	160458	216494	6.28%	0.652%
23	13.848	1952	1957	1960	rBV	1123230	1061433	30.77%	3.195%
24	13.871	1960	1961	1968	rVB	83997	71679	2.08%	0.216%
25	14.036	1985	1989	1992	rBV	104449	97468	2.83%	0.293%
26	14.342	2037	2041	2046	rVB	221369	213372	6.19%	0.642%
27	14.636	2087	2091	2098	rVV	459205	439459	12.74%	1.323%
28	14.706	2099	2103	2108	rVB	279393	271522	7.87%	0.817%
29	14.854	2125	2128	2132	rBV	64195	94179	2.73%	0.283%
30	14.954	2140	2145	2150	rBV	560348	628042	18.21%	1.890%
31	15.195	2182	2186	2191	rVB	66630	80178	2.32%	0.241%
32	15.254	2191	2196	2200	rBV	877767	1004393	29.12%	3.023%
33	15.306	2200	2205	2217	rVB	535584	698768	20.26%	2.103%
34	15.712	2268	2274	2280	rBV	365180	554872	16.08%	1.670%

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
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35	16.177	2347	2353	2362	rBV	182642	318202	9.22%	0.958%
36	16.595	2420	2424	2430	rBV3	27194	49210	1.43%	0.148%
37	16.724	2442	2446	2457	rVB3	76377	155437	4.51%	0.468%
38	17.000	2489	2493	2501	rVB2	23414	47461	1.38%	0.143%
39	17.365	2550	2555	2562	rVB4	30209	63460	1.84%	0.191%

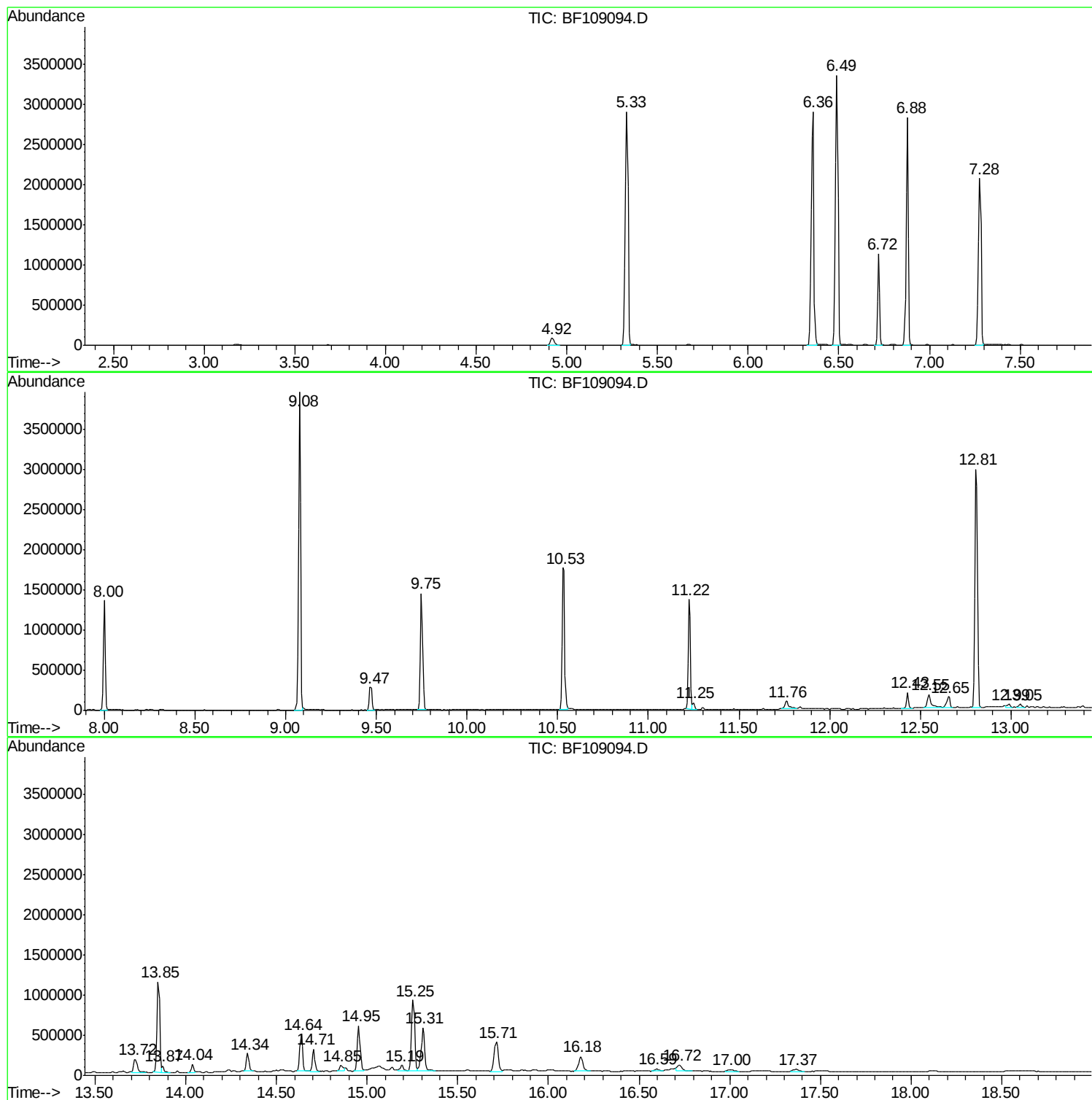
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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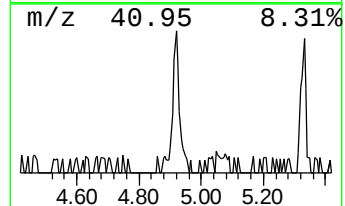
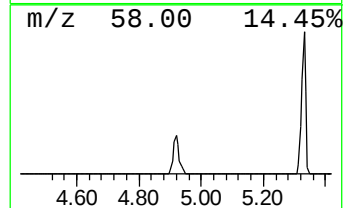
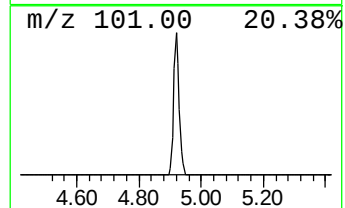
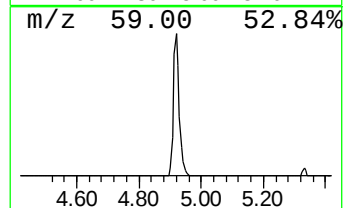
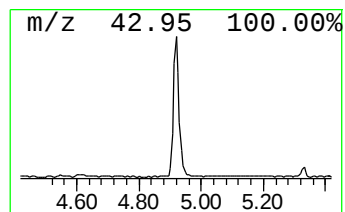
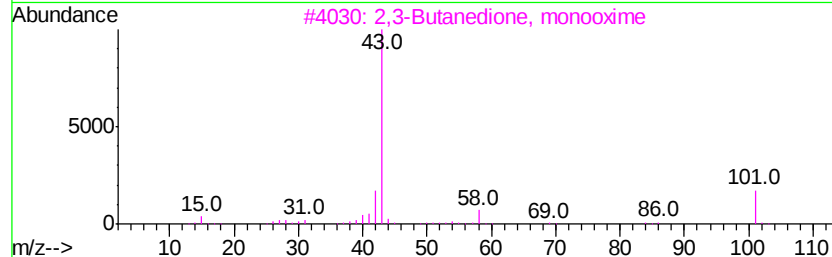
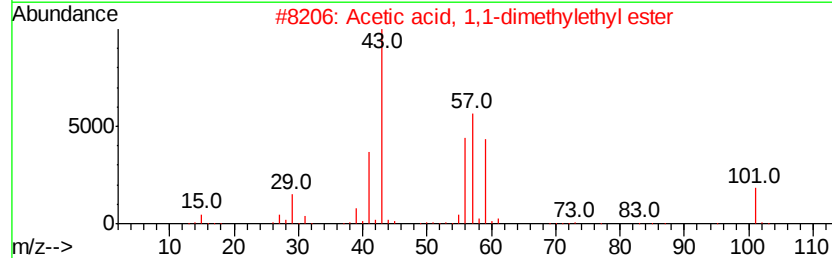
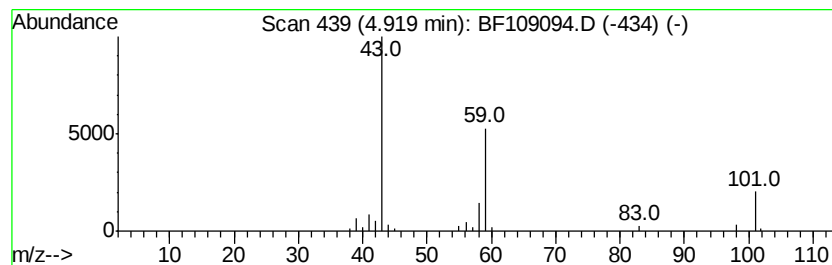
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	2.44 ng	107470	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Propylamine	59	C3H9N	000107-10-8	9



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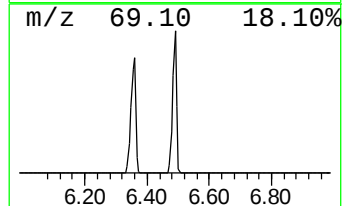
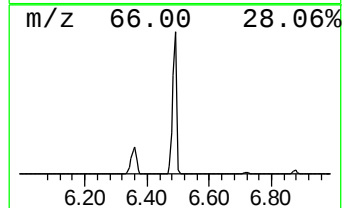
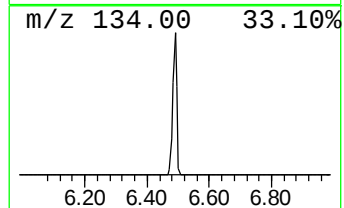
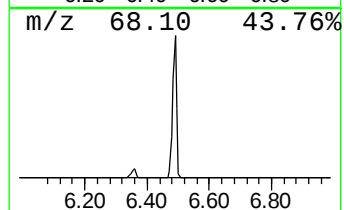
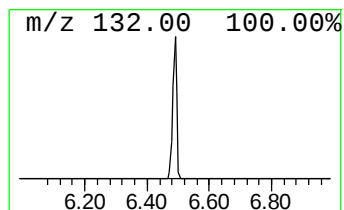
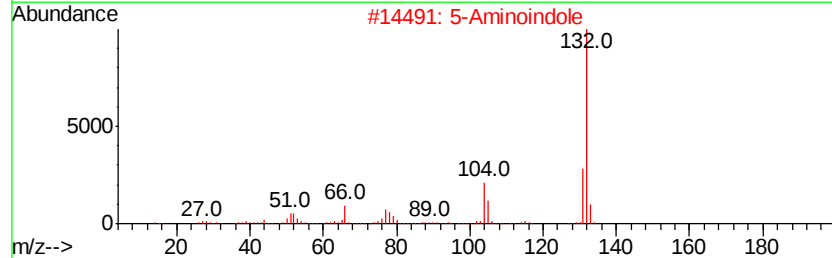
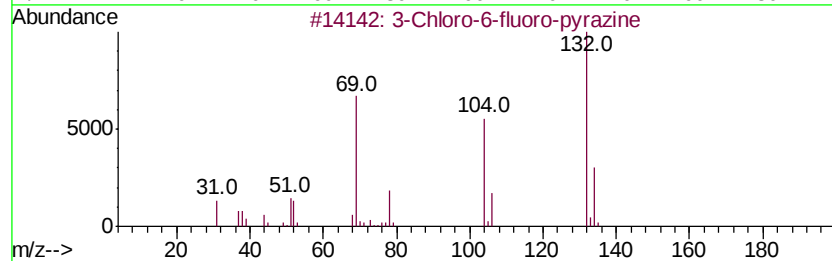
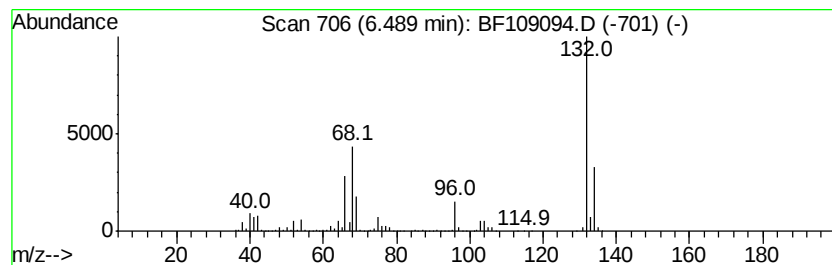
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.49	69.56 ng	3061340	1,4-Dichlorobenzene-d4	6.72

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4			Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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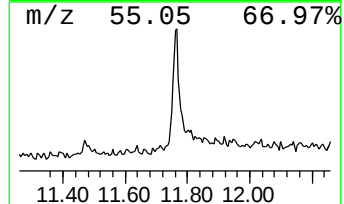
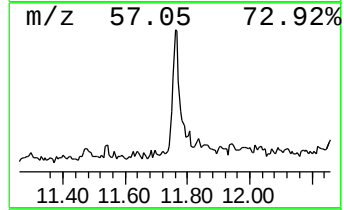
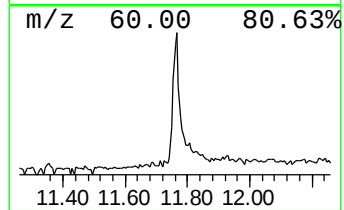
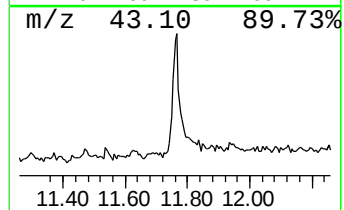
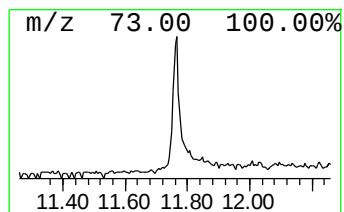
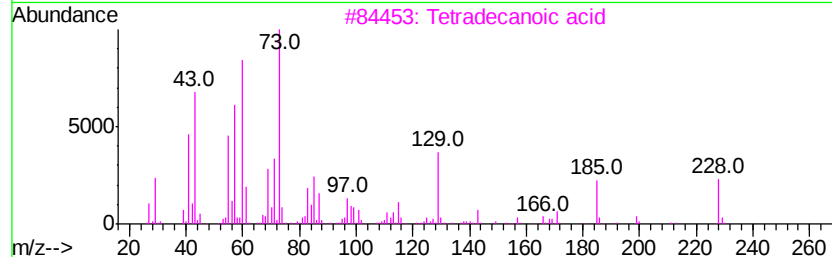
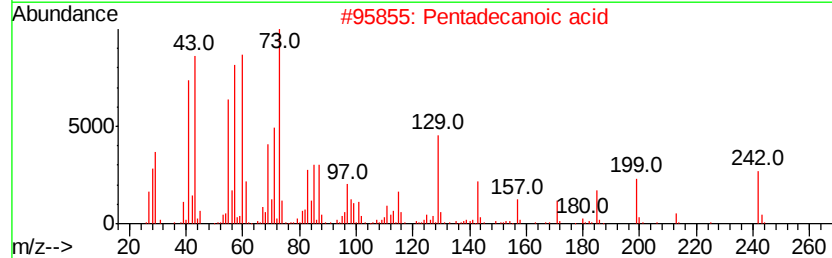
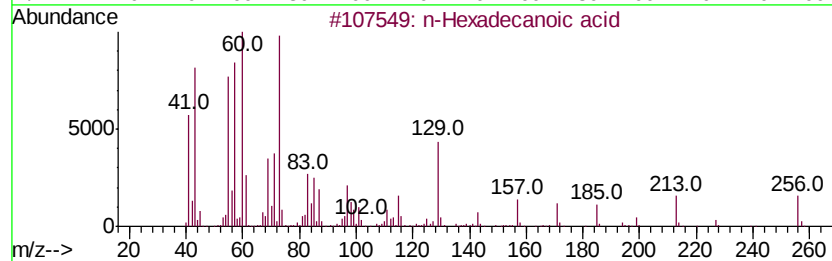
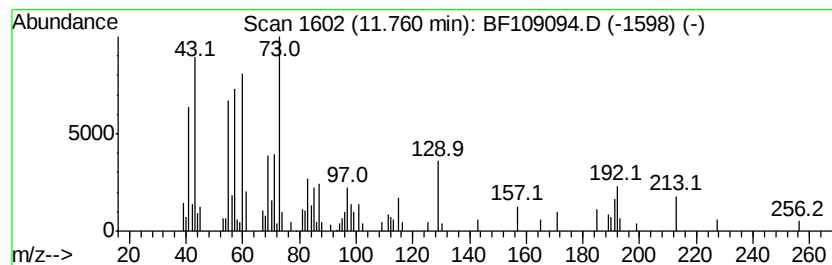
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.76	2.79 ng	170419	Phenanthrene-d10	11.22		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53



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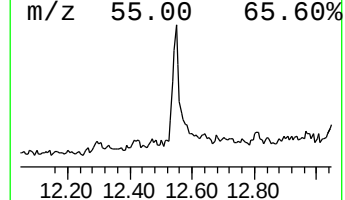
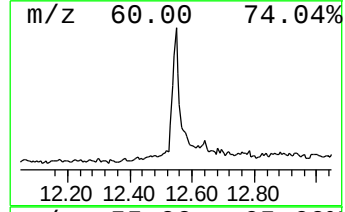
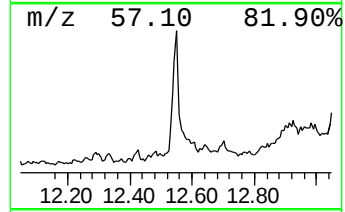
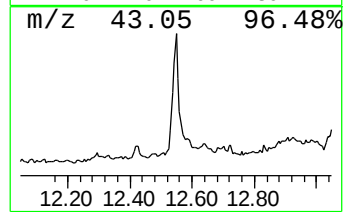
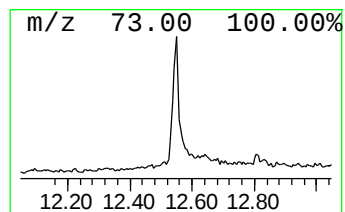
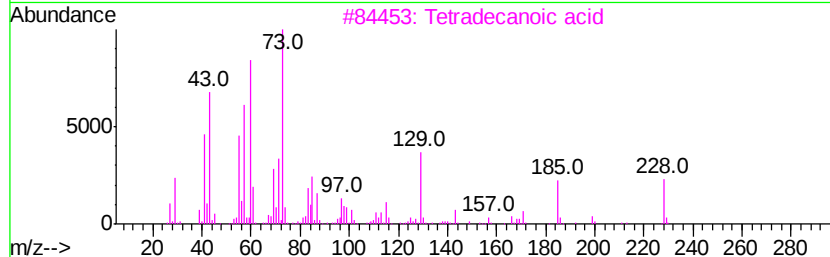
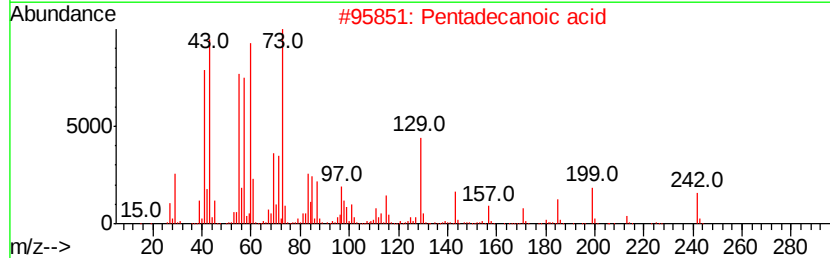
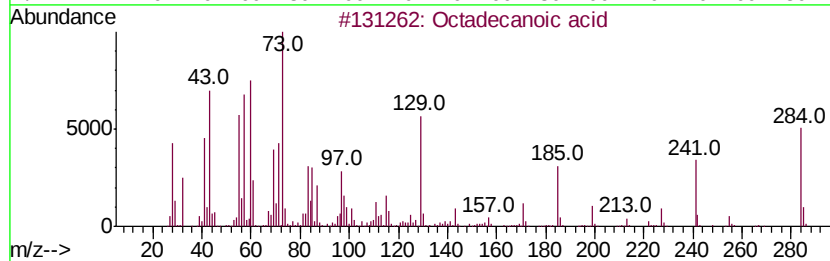
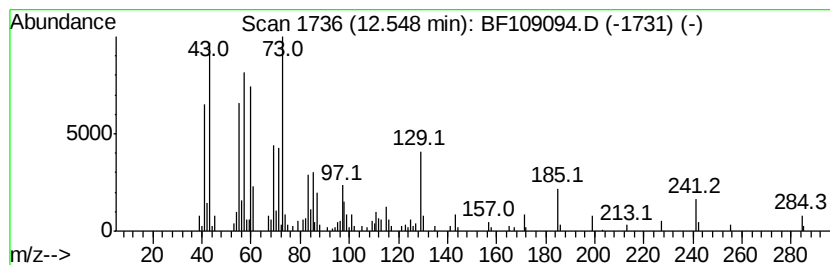
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.55	5.23 ng	277514	Chrysene-d12	13.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		n-Decanoic acid	172	C10H20O2	000334-48-5	68
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64



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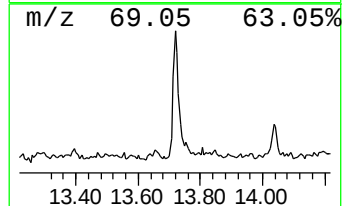
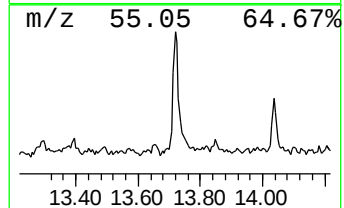
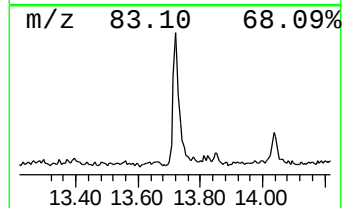
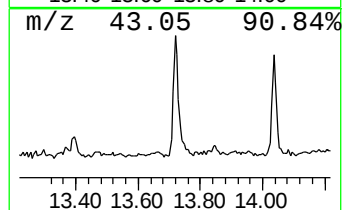
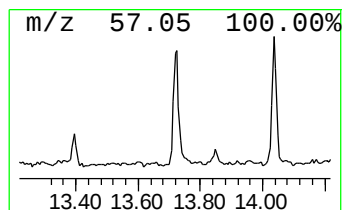
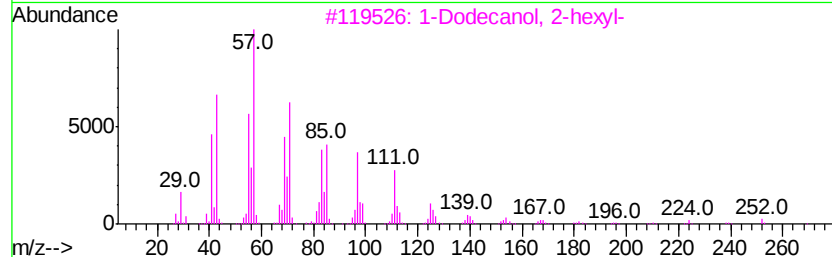
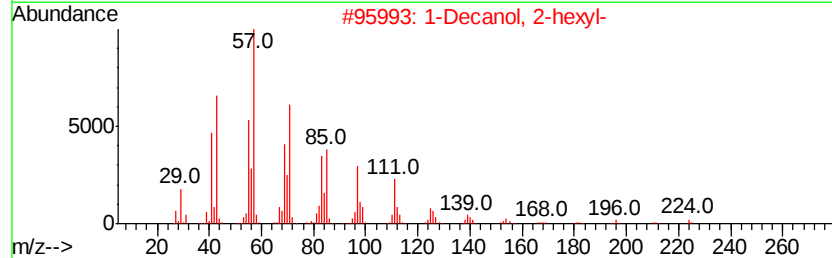
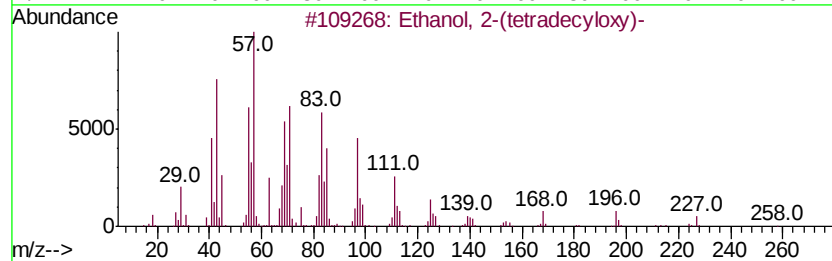
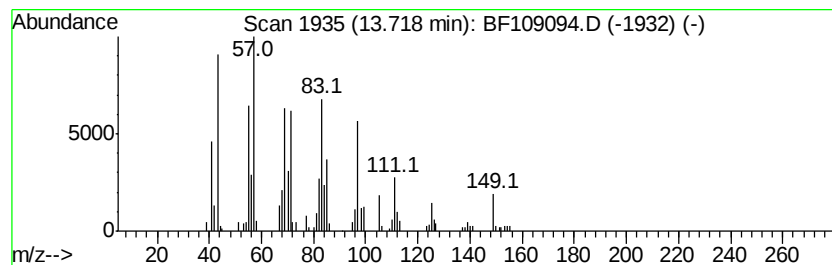
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 Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.08 ng	216494	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2		1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	70
3		1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	70
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	64
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	60



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Operator : JU/SJ
Sample : J4940-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

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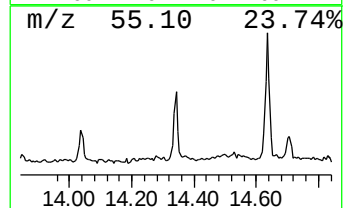
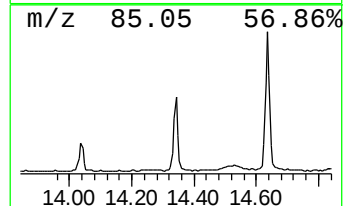
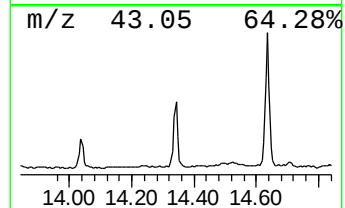
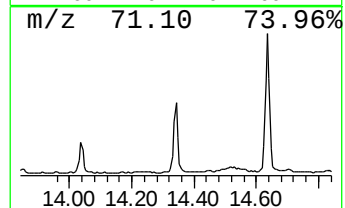
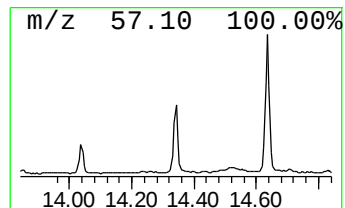
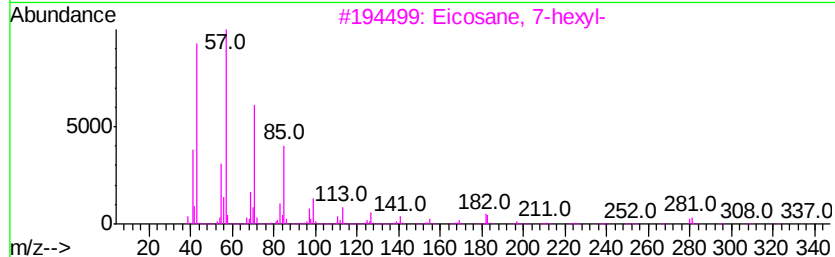
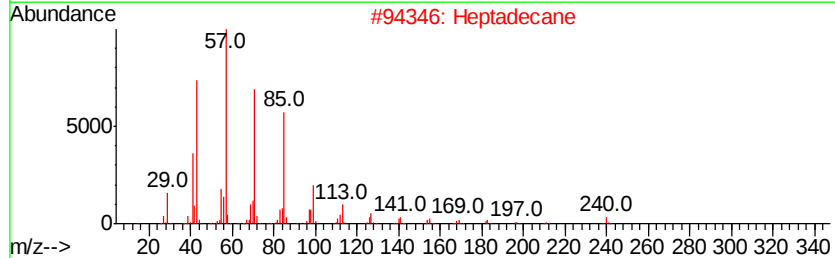
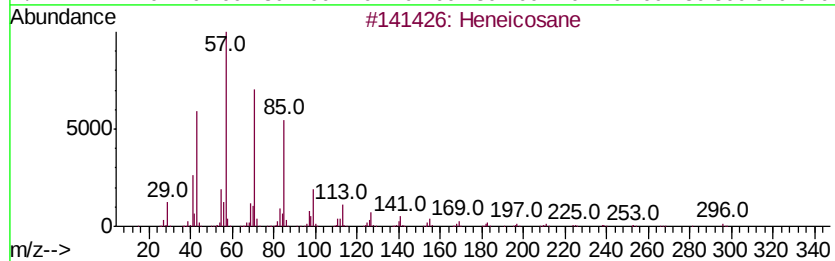
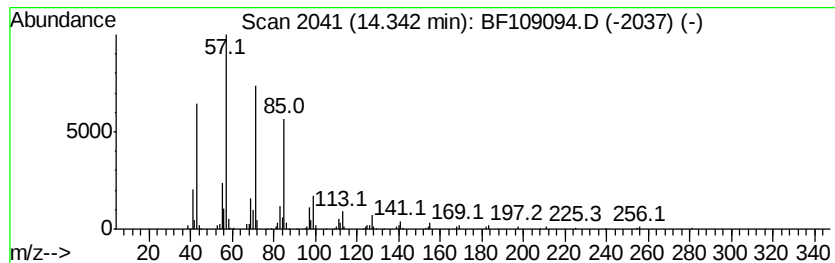
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.34	4.02 ng	213372	Chrysene-d12	13.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5		Hexacosane	366	C26H54	000630-01-3	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109094.D
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Instrument :
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ClientSampleId :
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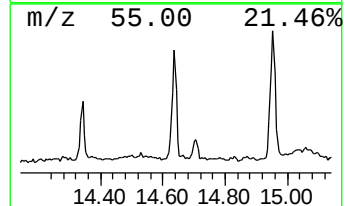
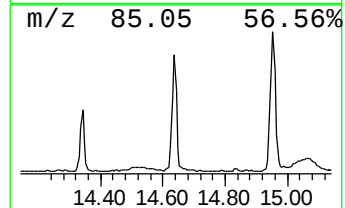
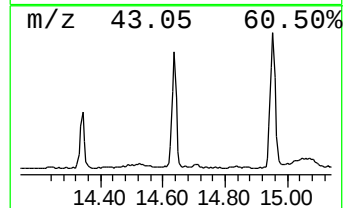
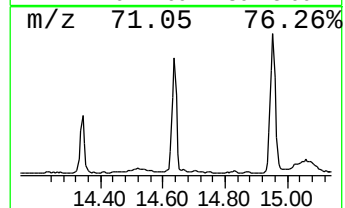
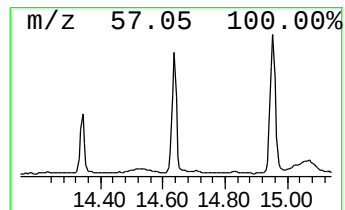
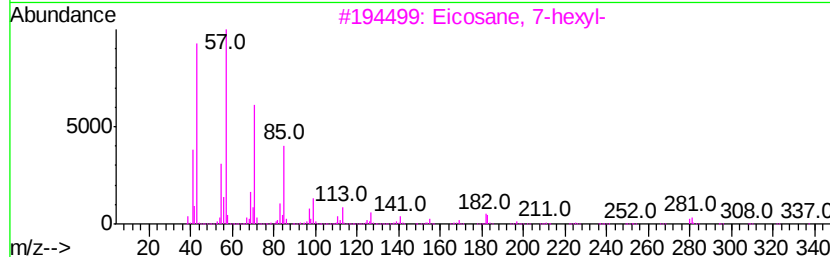
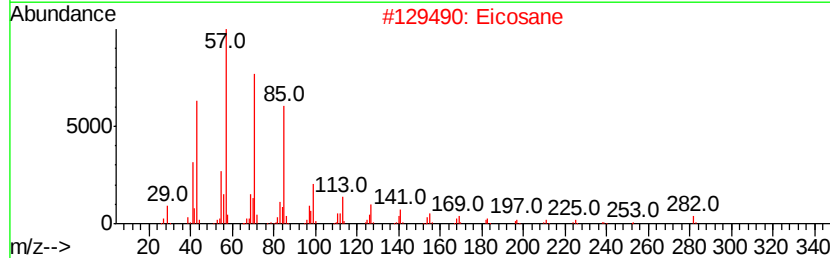
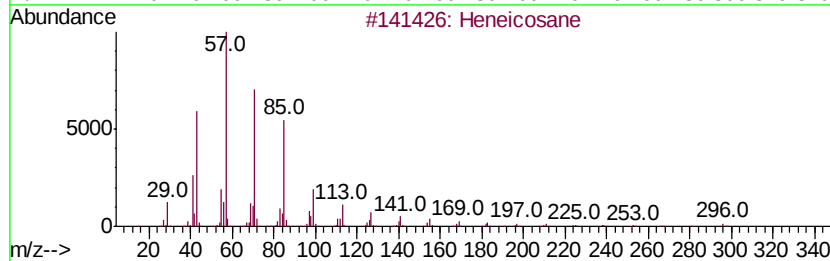
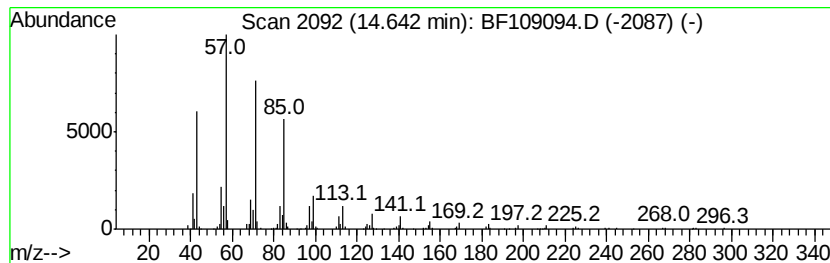
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	8.75 ng	439459	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	98
2		Eicosane	282	C20H42	000112-95-8	90
3		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
4		Hexadecane	226	C16H34	000544-76-3	87
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109094.D
Acq On : 18 Sep 2018 14:39
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Sample : J4940-01
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ALS Vial : 4 Sample Multiplier: 1

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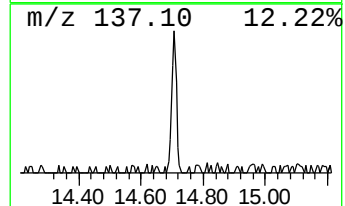
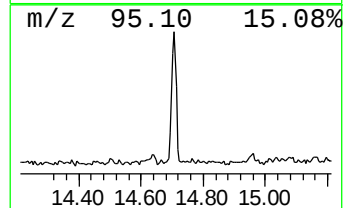
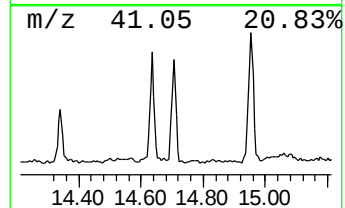
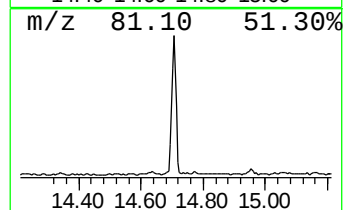
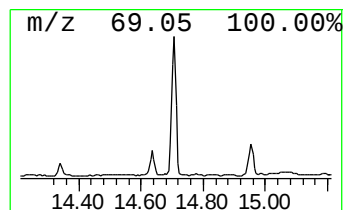
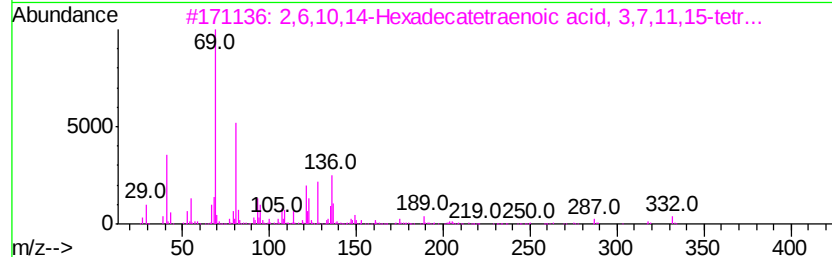
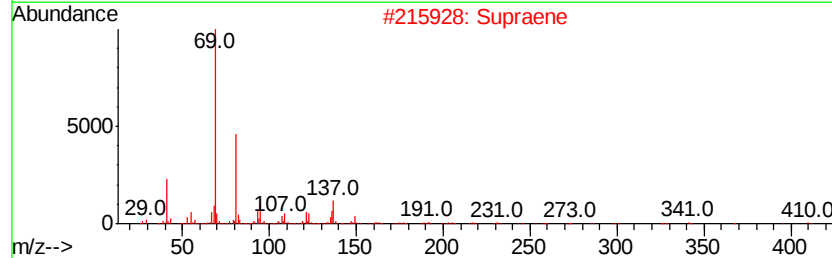
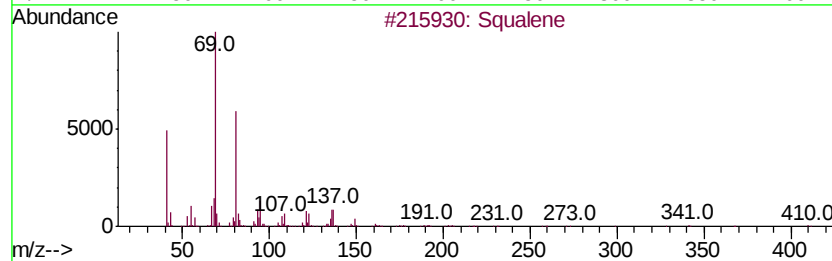
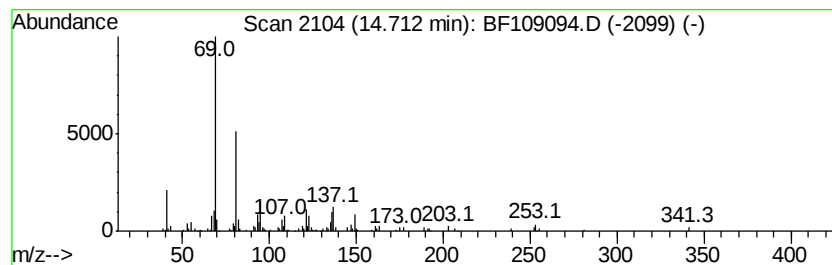
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.71	5.41 ng	271522	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4		(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109094.D
Acq On : 18 Sep 2018 14:39
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Misc :
ALS Vial : 4 Sample Multiplier: 1

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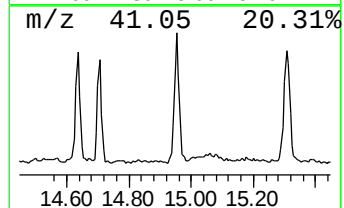
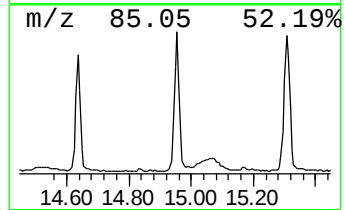
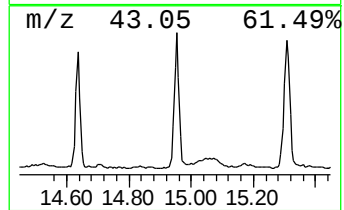
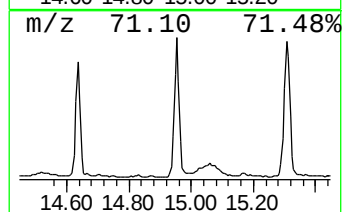
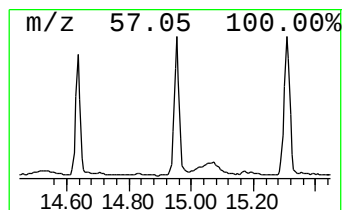
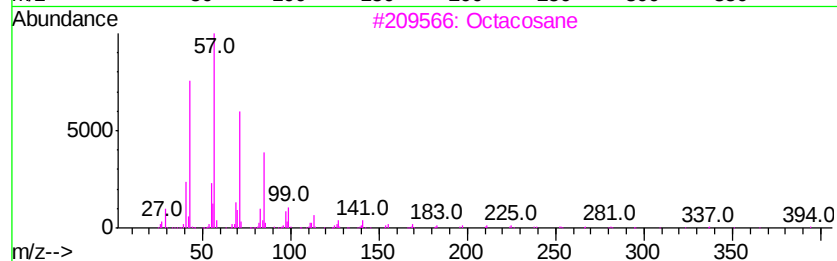
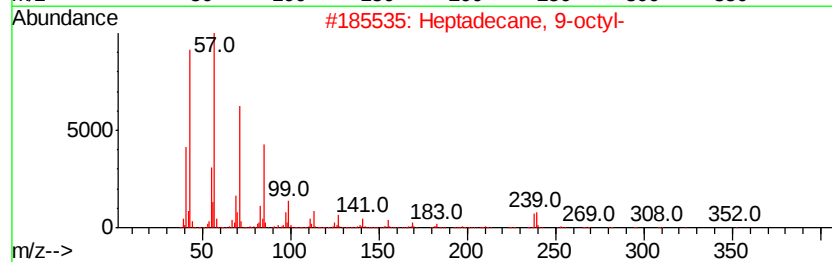
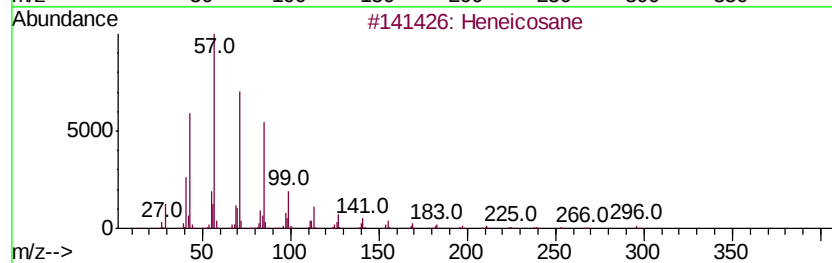
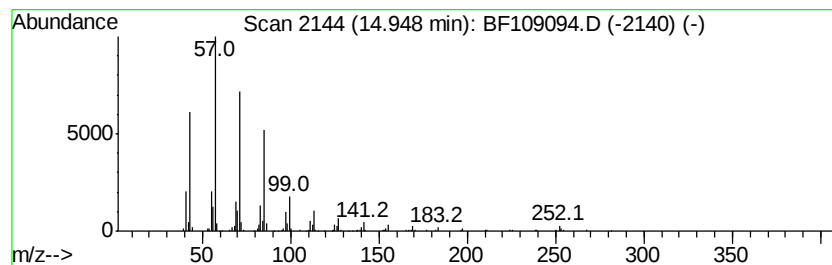
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.95	12.51 ng	628042	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
3		Octacosane	394	C28H58	000630-02-4	87
4		Tetratetracontane	619	C44H90	007098-22-8	87
5		Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109094.D
Acq On : 18 Sep 2018 14:39
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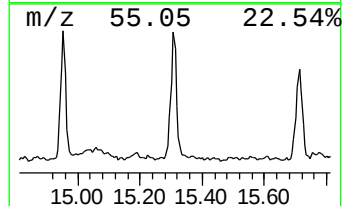
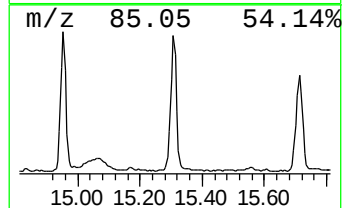
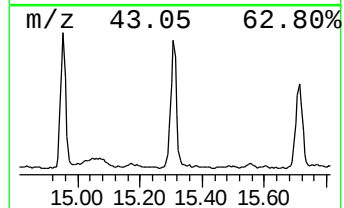
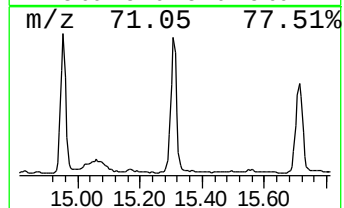
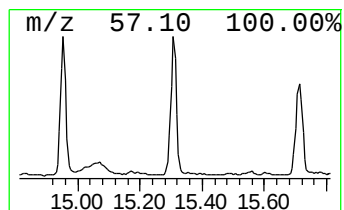
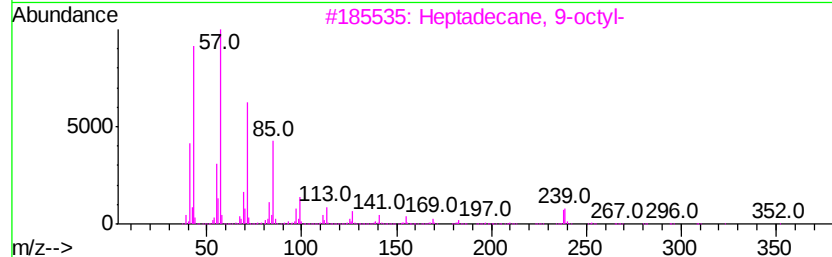
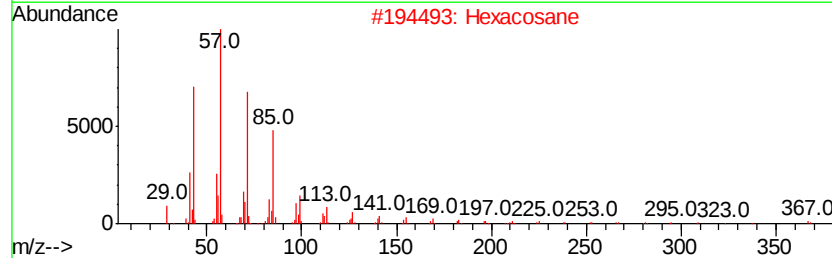
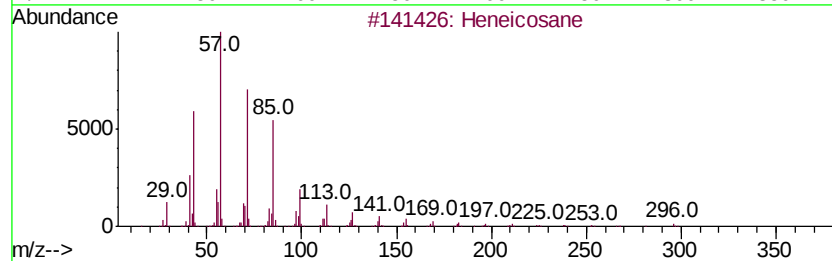
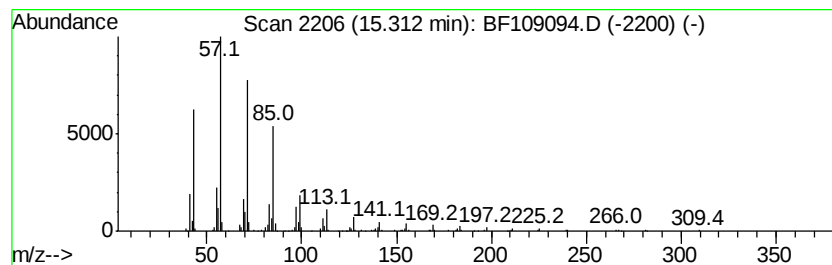
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.31	13.91 ng	698768	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	91
2		Hexacosane	366	C26H54	000630-01-3	91
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4		Eicosane	282	C20H42	000112-95-8	90
5		2-Bromotetradecane	276	C14H29Br	074036-95-6	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109094.D
Acq On : 18 Sep 2018 14:39
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Sample : J4940-01
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ClientSampleId :
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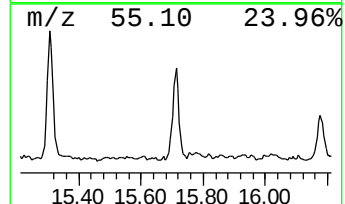
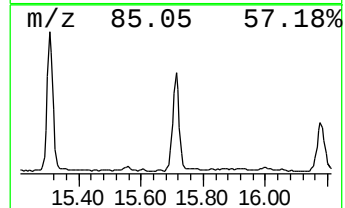
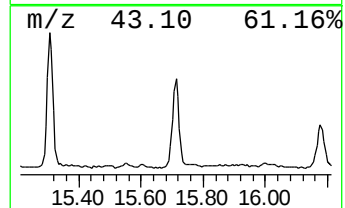
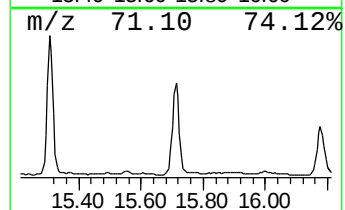
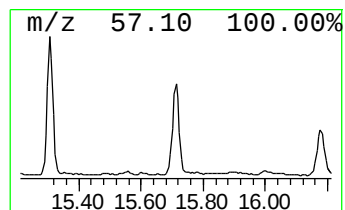
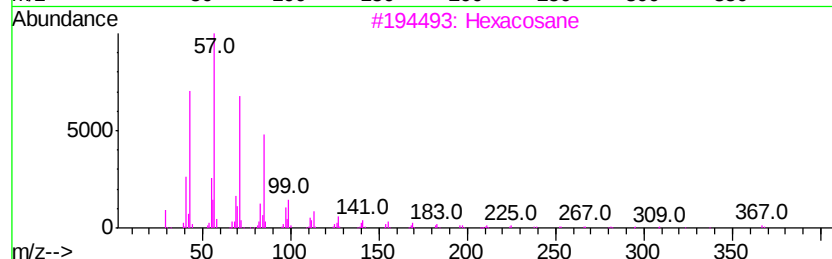
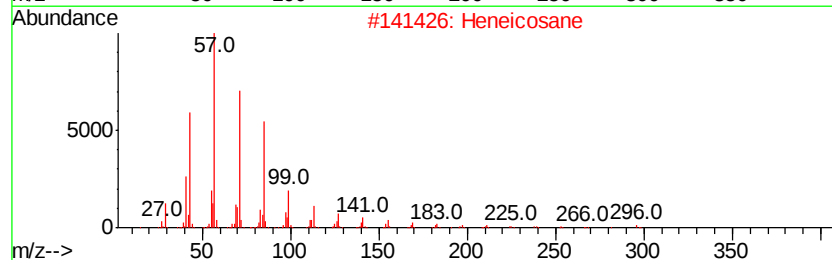
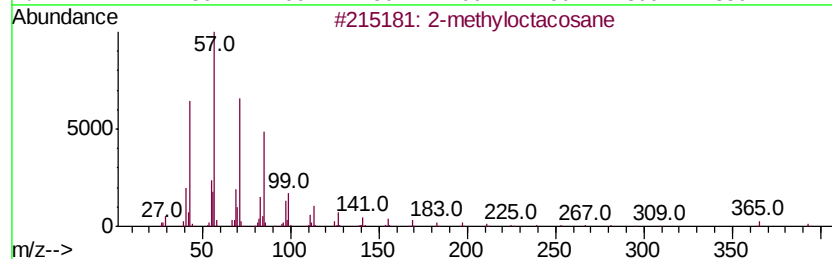
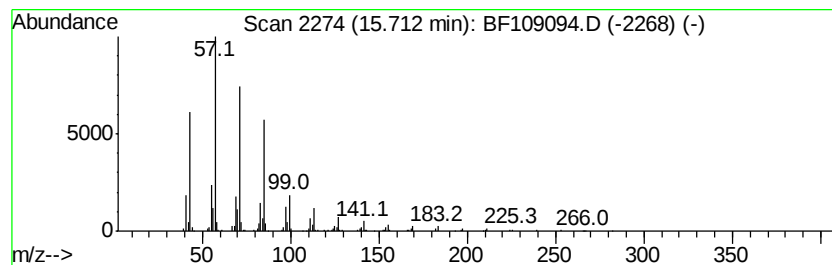
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2-methyloctacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.71	11.05 ng	554872	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Heptadecane	240	C17H36	000629-78-7	91
5		Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
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ClientSampleId :
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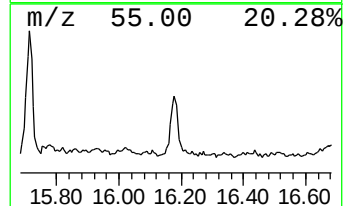
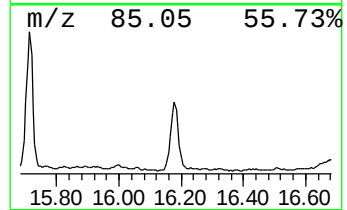
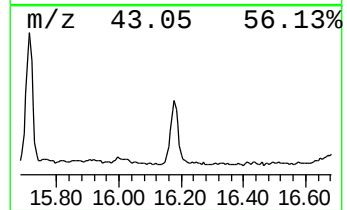
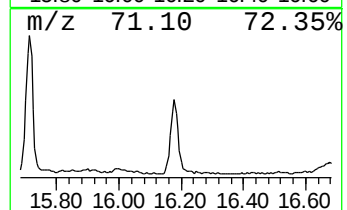
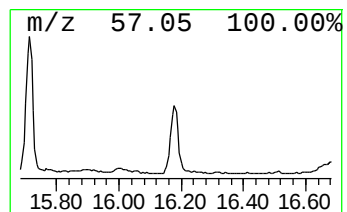
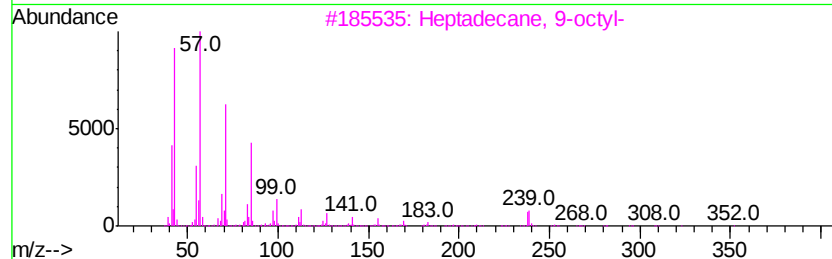
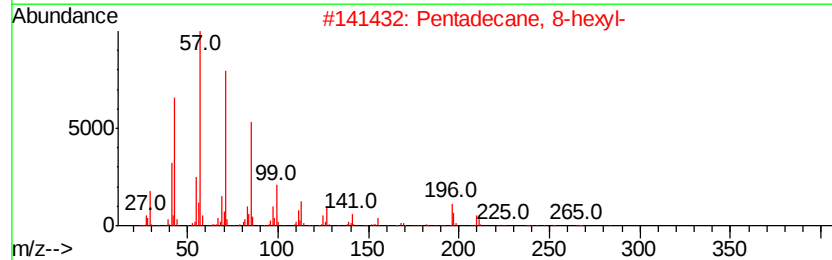
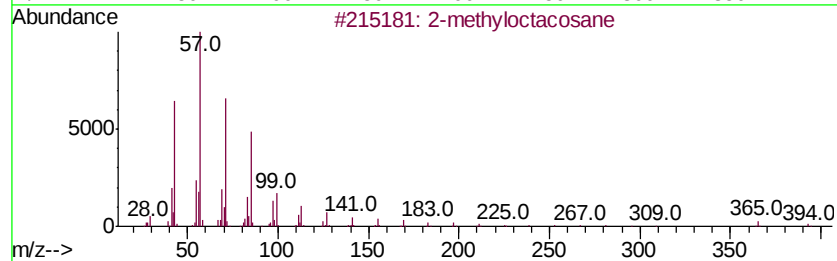
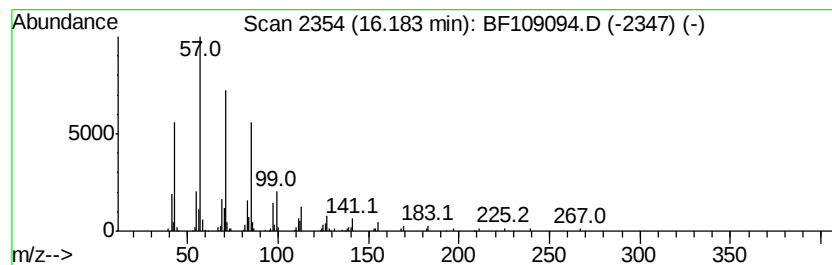
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentadecane, 8-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.18	6.34 ng	318202	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-methyloctacosane	408	C29H60	1000376-72-8	91
2		Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	90
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
4		Octadecane	254	C18H38	000593-45-3	87
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091818\
Data File : BF109094.D
Acq On : 18 Sep 2018 14:39
Operator : JU/SJ
Sample : J4940-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

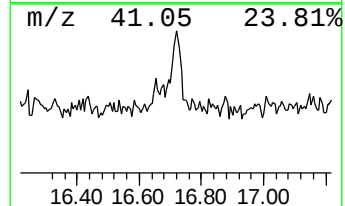
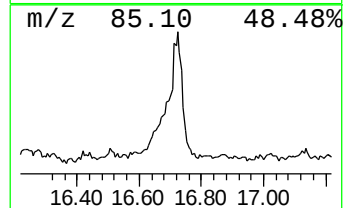
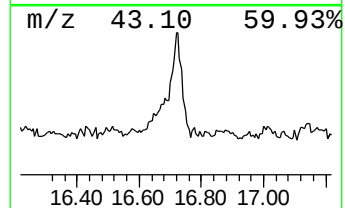
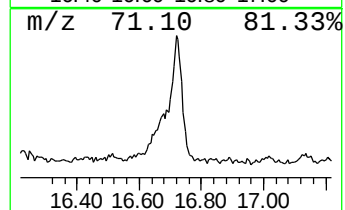
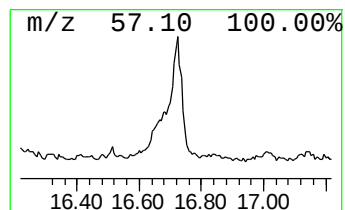
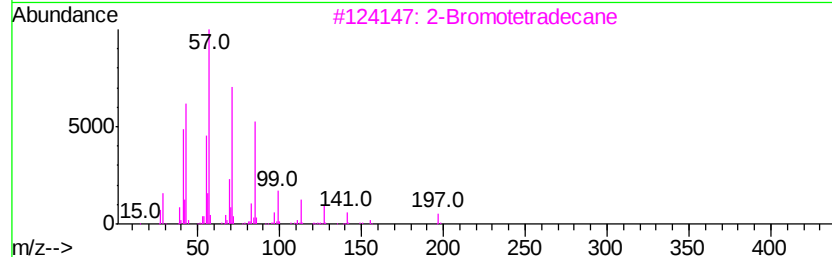
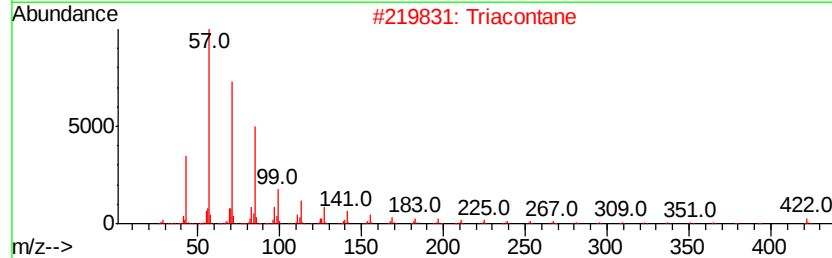
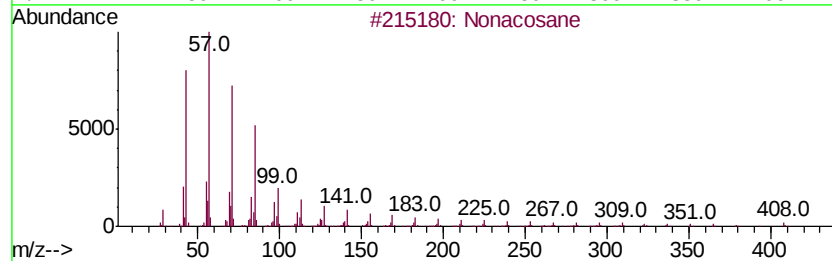
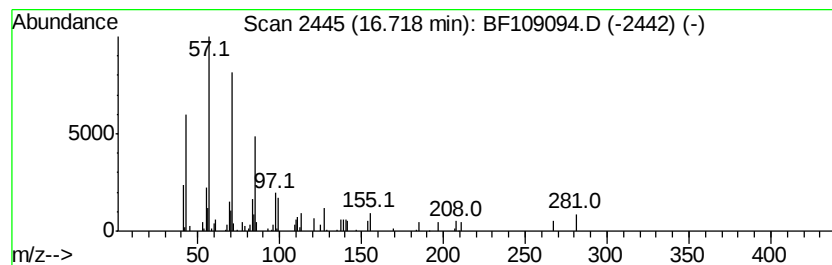
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF091418.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Nonacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	3.10 ng	155437	Perylene-d12	15.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonacosane	408	C29H60	000630-03-5	86
2		triacontane	422	C30H62	000638-68-6	80
3		2-Bromotetradecane	276	C14H29Br	074036-95-6	80
4		2-methyloctacosane	408	C29H60	1000376-72-8	78
5		Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091818\
Data File : BF109094.D
Acq On : 18 Sep 2018 14:39
Operator : JU/SJ
Sample : J4940-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
COMP-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091418.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...	4.92	2.4	ng	107470	1	6.72	880200	20.0
unknown6.49	6.49	69.6	ng	3061340	1	6.72	880200	20.0
n-Hexadecanoic acid	11.76	2.8	ng	170419	4	11.22	1221270	20.0
Octadecanoic acid	12.55	5.2	ng	277514	5	13.85	1061430	20.0
Ethanol, 2-(tetra...	13.72	4.1	ng	216494	5	13.85	1061430	20.0
Heptadecane	14.34	4.0	ng	213372	5	13.85	1061430	20.0
Heneicosane	14.64	8.8	ng	439459	6	15.25	1004390	20.0
Squalene	14.71	5.4	ng	271522	6	15.25	1004390	20.0
Heptadecane, 9-oc...	14.95	12.5	ng	628042	6	15.25	1004390	20.0
Eicosane	15.31	13.9	ng	698768	6	15.25	1004390	20.0
2-methyloctacosane	15.71	11.1	ng	554872	6	15.25	1004390	20.0
Pentadecane, 8-he...	16.18	6.3	ng	318202	6	15.25	1004390	20.0
Nonacosane	16.72	3.1	ng	155437	6	15.25	1004390	20.0