

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF062217\
 Data File : BF096127.D
 Acq On : 22 Jun 2017 17:54
 Operator : SJ/MA
 Sample : I3775-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHD-SB-020304-0-11

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:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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	1.546	8	10	51	rVB	811227	1650422	87.18%	8.785%
2	2.257	128	131	136	rBV2	13133	29704	1.57%	0.158%
3	4.445	499	503	521	rBV2	85730	254066	13.42%	1.352%
4	4.822	561	567	575	rBV2	10060	19828	1.05%	0.106%
5	5.163	622	625	649	rBV	662631	1600784	84.56%	8.520%
6	5.398	661	665	679	rVB	106404	181966	9.61%	0.969%
7	6.857	909	913	923	rBV	744778	1361665	71.93%	7.248%
8	6.939	923	927	949	rVB	1006144	1893162	100.00%	10.077%
9	7.275	980	984	997	rBV	288399	394496	20.84%	2.100%
10	7.510	1019	1024	1042	rBV	930467	1272085	67.19%	6.771%
11	8.198	1137	1141	1166	rBV	565482	934934	49.38%	4.976%
12	9.310	1326	1330	1352	rBV	359547	554311	29.28%	2.950%
13	11.092	1627	1633	1654	rBV	1406192	1778288	93.93%	9.465%
14	11.792	1747	1752	1763	rBV	252395	339430	17.93%	1.807%
15	11.916	1769	1773	1781	rVB	18085	27043	1.43%	0.144%
16	12.133	1805	1810	1815	rBV2	409800	530781	28.04%	2.825%
17	12.180	1815	1818	1824	rVV2	24342	35077	1.85%	0.187%
18	12.992	1952	1956	1959	rVV	27763	30370	1.60%	0.162%
19	13.039	1959	1964	1973	rVB3	16365	29934	1.58%	0.159%
20	13.351	2004	2017	2021	rBV5	9457	25844	1.37%	0.138%
21	13.433	2027	2031	2045	rBV	500386	772240	40.79%	4.110%
22	13.762	2082	2087	2094	rBV2	28550	52929	2.80%	0.282%
23	14.492	2206	2211	2213	rBV2	20963	24189	1.28%	0.129%
24	14.527	2213	2217	2221	rVV	349924	460992	24.35%	2.454%
25	14.568	2221	2224	2236	rVB	110641	165407	8.74%	0.880%
26	14.668	2237	2241	2247	rVV	24699	37768	1.99%	0.201%
27	15.345	2353	2356	2360	rBV	18314	24322	1.28%	0.129%
28	15.392	2360	2364	2368	rVB2	20916	26431	1.40%	0.141%
29	15.492	2379	2381	2386	rVV3	29932	43942	2.32%	0.234%
30	15.557	2388	2392	2399	rVB5	35630	60647	3.20%	0.323%
31	15.804	2426	2434	2438	rBV2	12691	25070	1.32%	0.133%
32	16.204	2498	2502	2506	rVV4	17152	21185	1.12%	0.113%
33	16.362	2524	2529	2536	rBV	200863	251282	13.27%	1.337%
34	16.503	2549	2553	2556	rBV	17113	21661	1.14%	0.115%

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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	16.662	2576	2580	2587	rBV	191119	263372	13.91%	1.402%
36	16.915	2618	2623	2630	rVV	1007522	1181664	62.42%	6.290%
37	16.992	2630	2636	2643	rVB6	14546	35256	1.86%	0.188%
38	17.103	2651	2655	2658	rBV4	13964	21946	1.16%	0.117%
39	17.145	2658	2662	2667	rVB	38175	55575	2.94%	0.296%
40	17.227	2672	2676	2680	rVB	33076	44118	2.33%	0.235%
41	17.280	2681	2685	2689	rBV2	20300	30535	1.61%	0.163%
42	17.392	2699	2704	2706	rBV3	12533	19417	1.03%	0.103%
43	18.045	2811	2815	2821	rVB2	47506	65132	3.44%	0.347%
44	18.174	2834	2837	2845	rBV3	52533	79381	4.19%	0.423%
45	18.262	2847	2852	2857	rBV2	388029	573904	30.31%	3.055%
46	18.303	2857	2859	2863	rVB	48635	51282	2.71%	0.273%
47	18.439	2879	2882	2885	rBV	39754	35699	1.89%	0.190%
48	18.480	2885	2889	2895	rBV2	135222	222893	11.77%	1.186%
49	18.568	2901	2904	2908	rBV3	20449	23846	1.26%	0.127%
50	18.892	2954	2959	2963	rBV	207298	235262	12.43%	1.252%
51	19.303	3024	3029	3034	rBV	149266	191971	10.14%	1.022%
52	19.544	3066	3070	3073	rBV	103630	142463	7.53%	0.758%
53	19.662	3087	3090	3093	rBV	22947	27384	1.45%	0.146%
54	19.833	3116	3119	3125	rBV	59200	85164	4.50%	0.453%
55	19.892	3126	3129	3134	rVV	80431	97202	5.13%	0.517%
56	19.944	3134	3138	3147	rBV	253933	372126	19.66%	1.981%

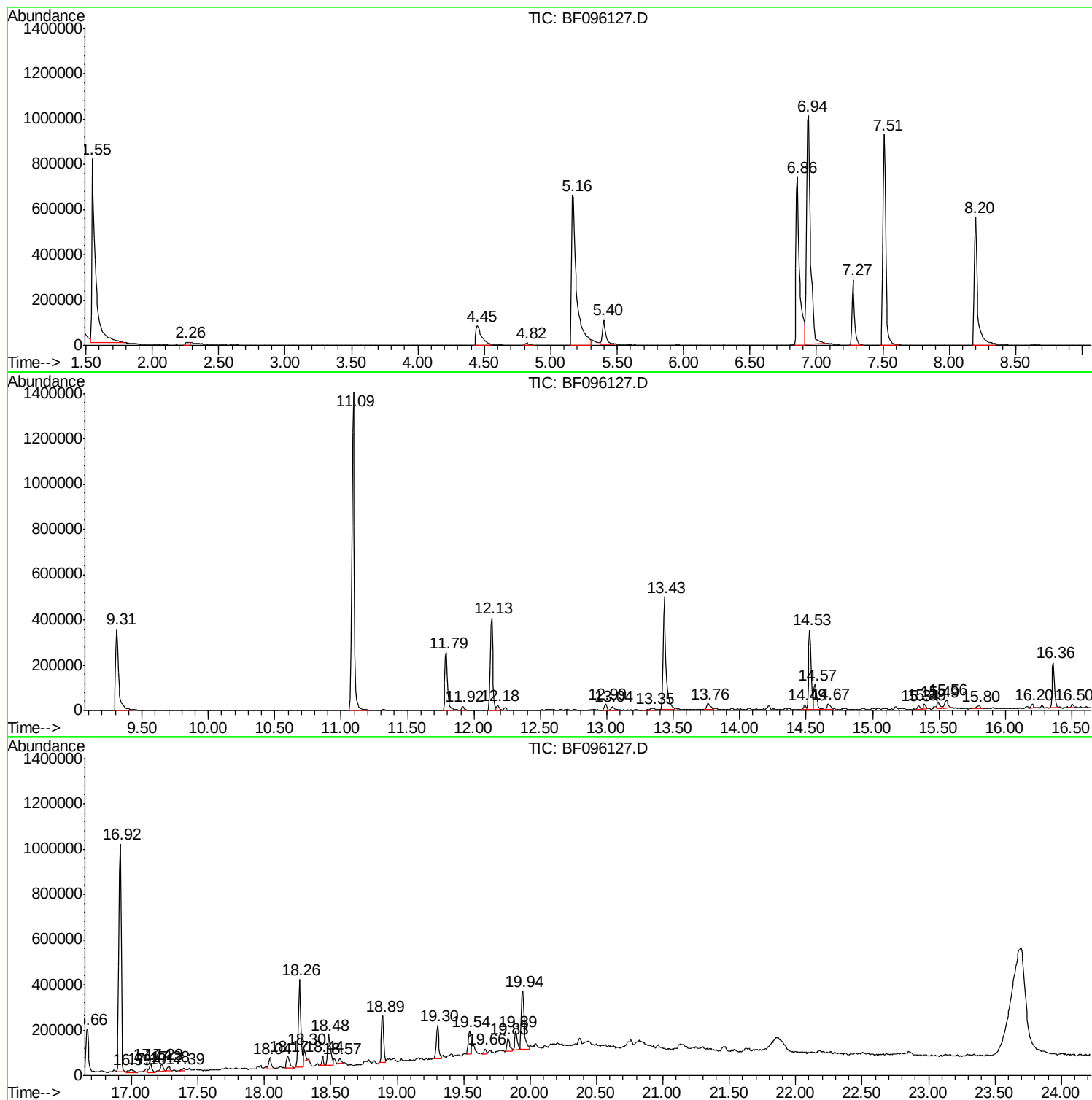
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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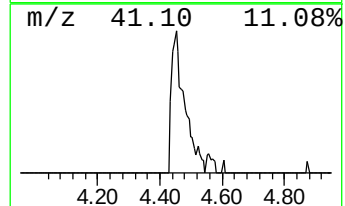
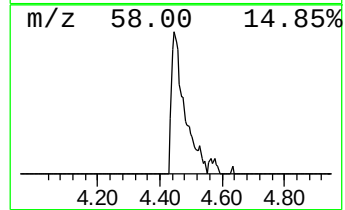
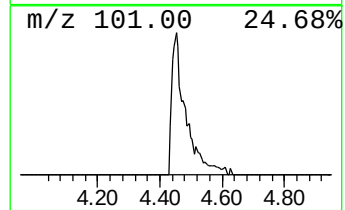
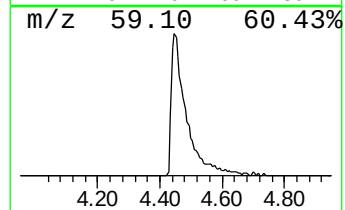
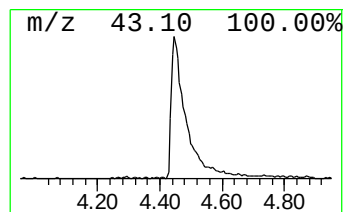
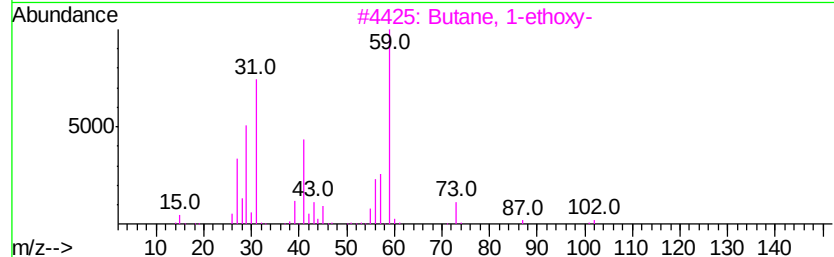
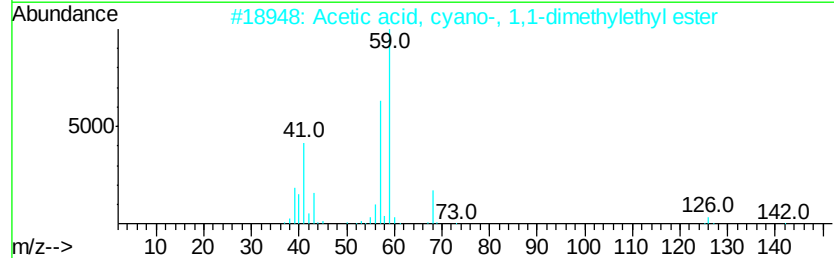
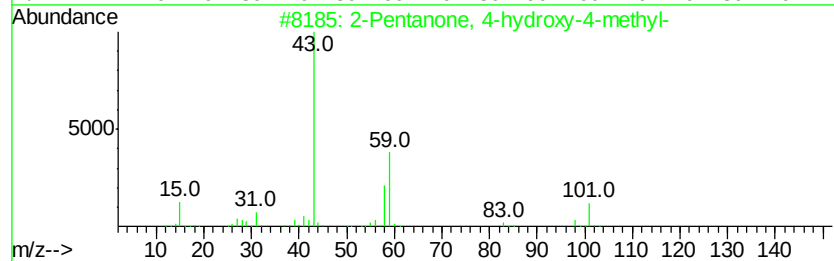
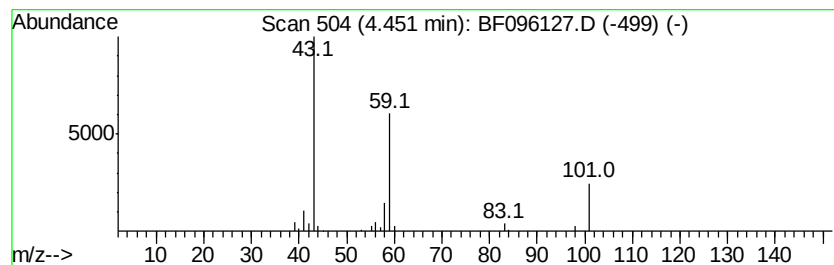
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	12.88 ng	254066	1,4-Dichlorobenzene-d4	7.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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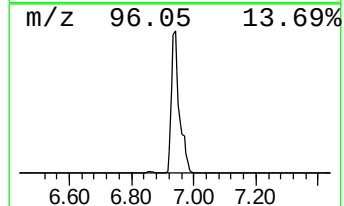
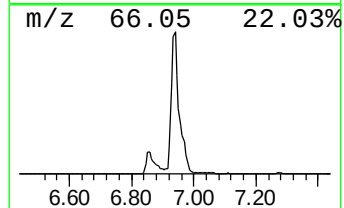
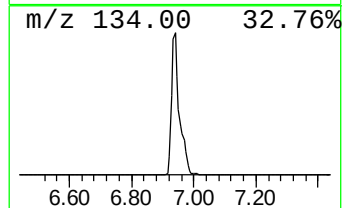
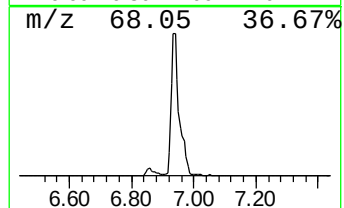
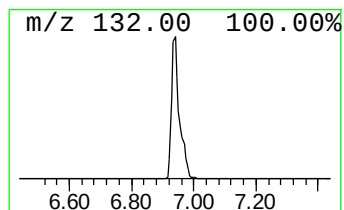
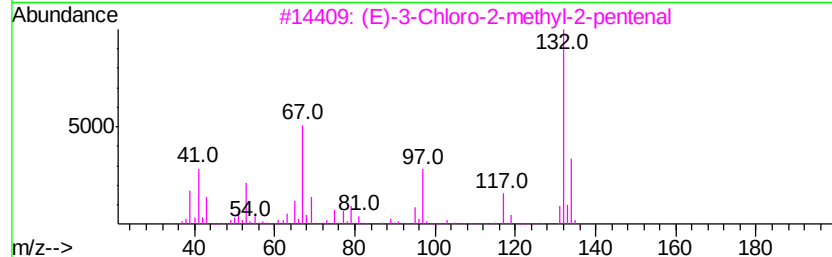
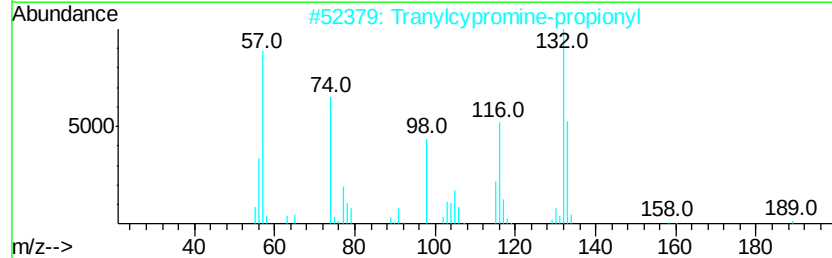
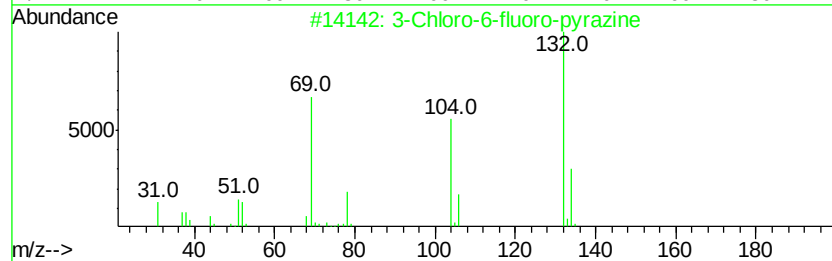
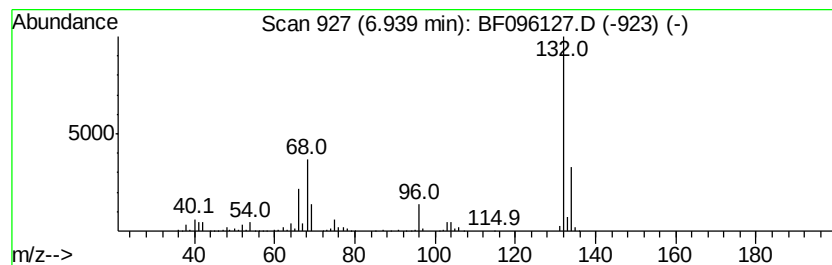
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Peak Number 4 unknown6.94 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	95.98 ng	1893160	1,4-Dichlorobenzene-d4	7.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Xenon	132	Xe	007440-63-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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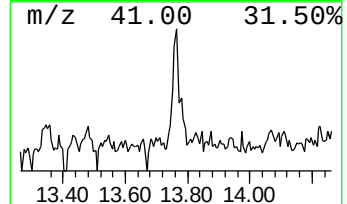
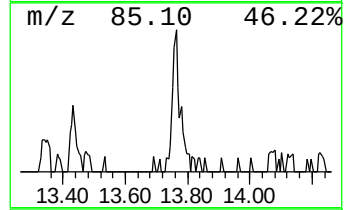
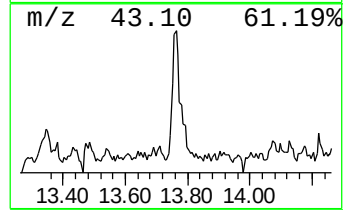
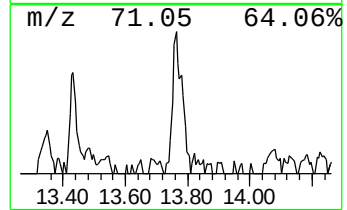
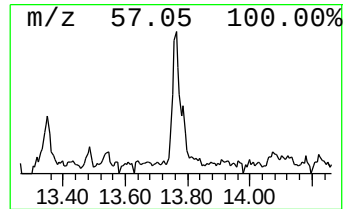
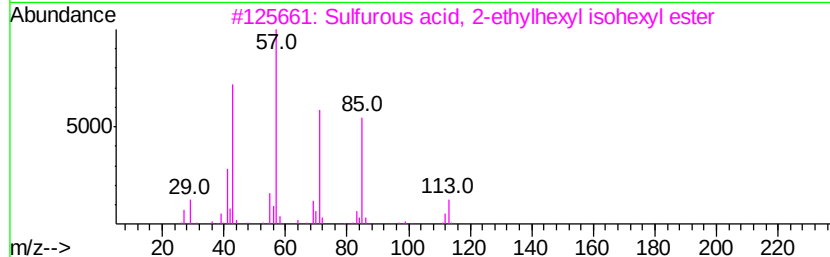
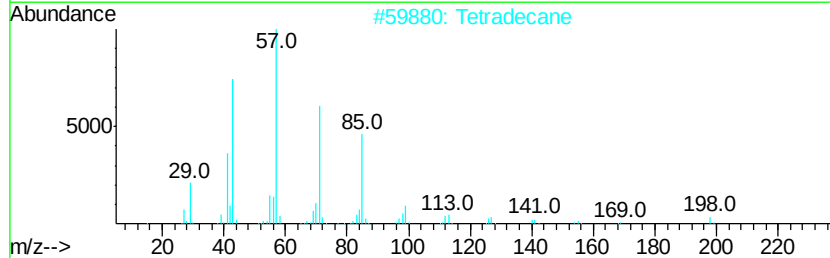
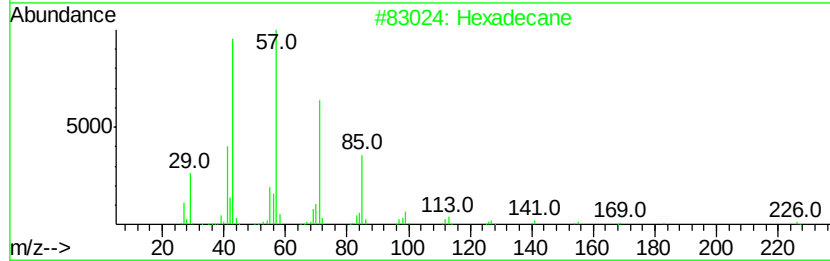
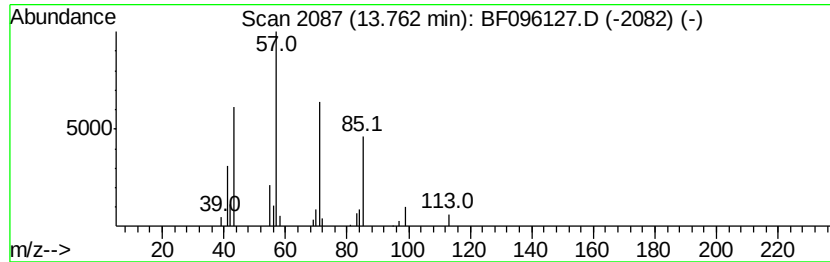
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.76	2.30 ng	52929	Phenanthrene-d10	14.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	83
2	Tetradecane	198	C14H30	000629-59-4	83
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	78
4	Pentadecane	212	C15H32	000629-62-9	78
5	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	72



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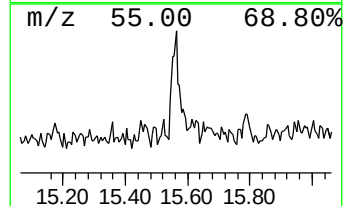
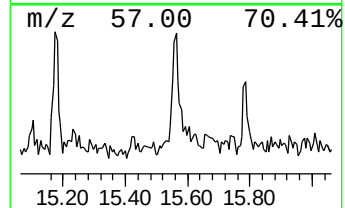
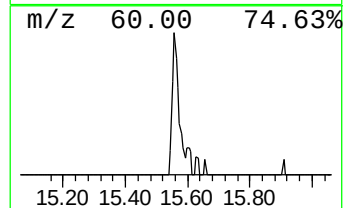
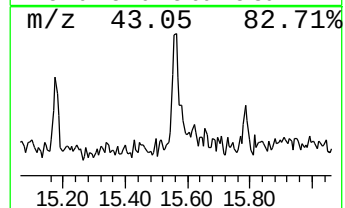
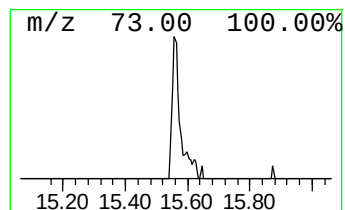
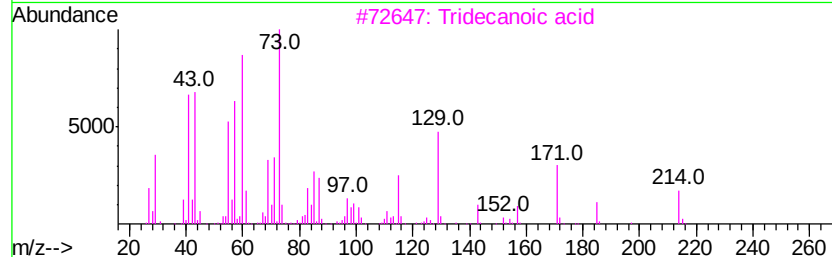
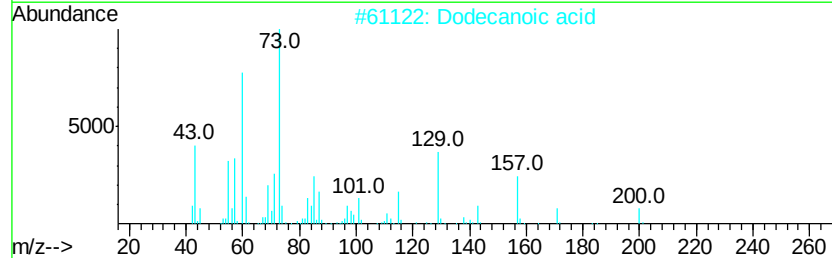
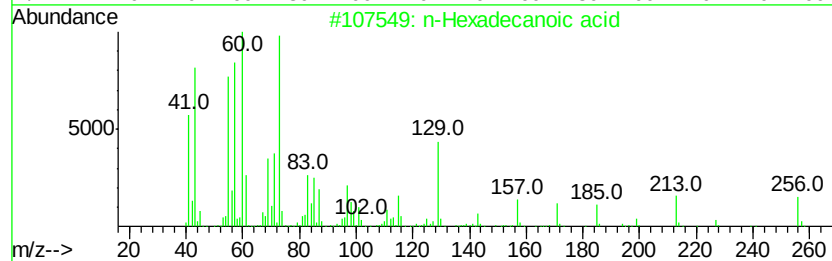
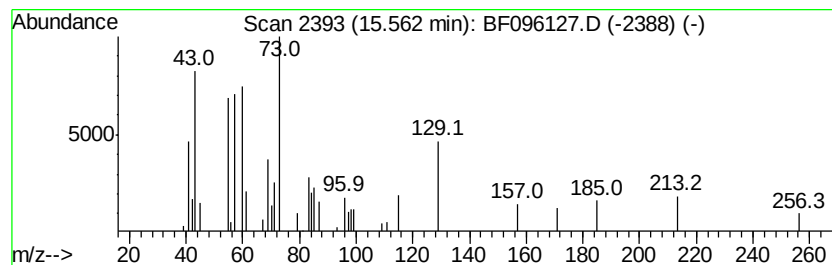
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.	
15.56	2.63 ng	60647	Phenanthrene-d10		14.53	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Dodecanoic acid	200	C12H24O2	000143-07-7	58
3		Tridecanoic acid	214	C13H26O2	000638-53-9	58
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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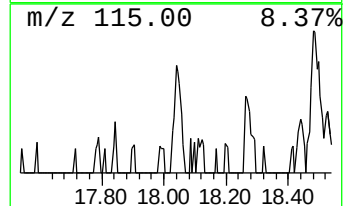
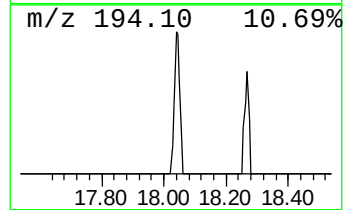
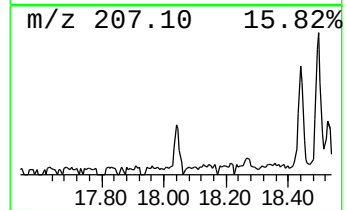
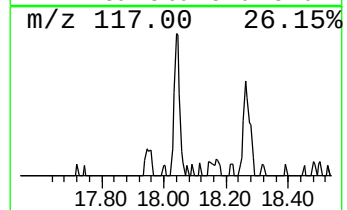
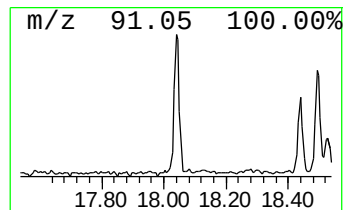
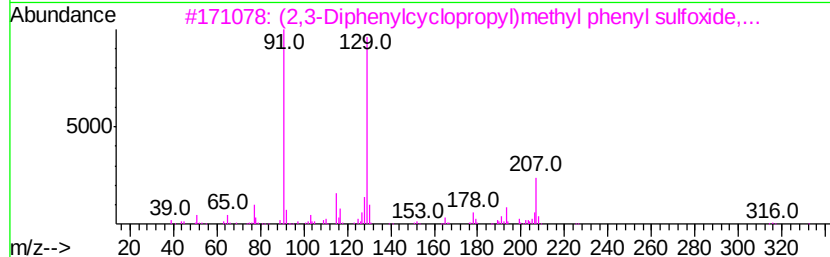
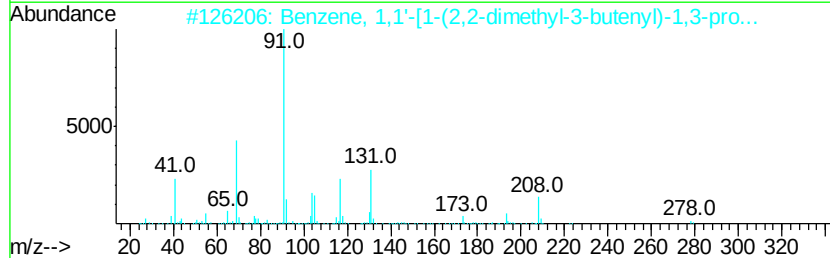
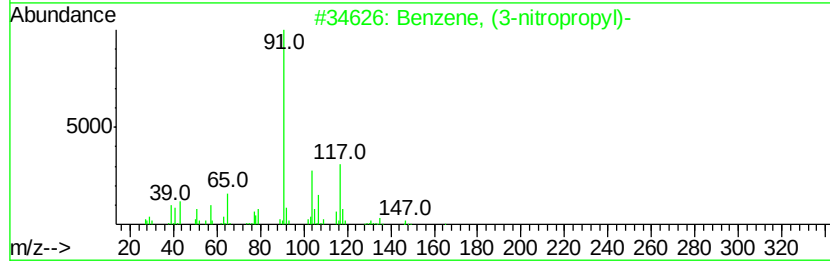
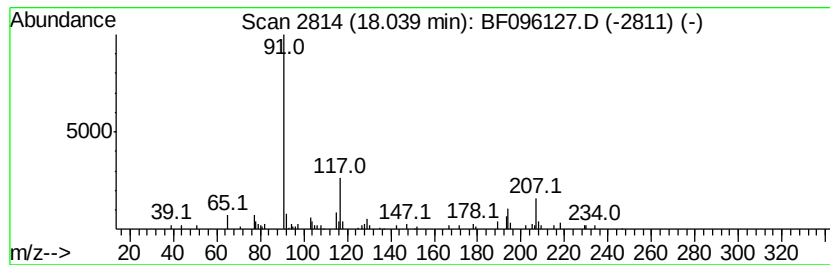
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ClientSampleId :
GHD-SB-020304-0-11

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown18.04 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.04	2.27 ng	65132	Chrysene-d12	18.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (3-nitropropyl)-	165	C9H11NO2	022818-69-5	25
2	Benzene, 1,1'-[1-(2,2-dimethyl-3...	278	C21H26	061142-62-9	23
3	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	12
4	Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	12
5	4-Benzyloxypyridazine 1-oxide	202	C11H10N2O2	002096-53-9	11



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF062217\
Data File : BF096127.D
Acq On : 22 Jun 2017 17:54
Operator : SJ/MA
Sample : I3775-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

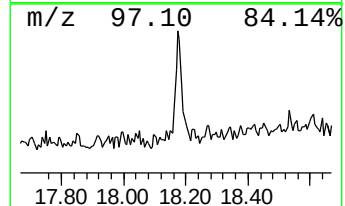
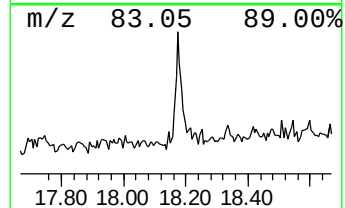
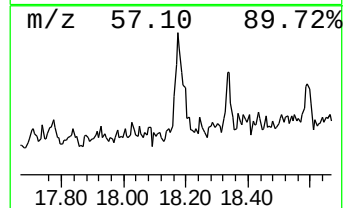
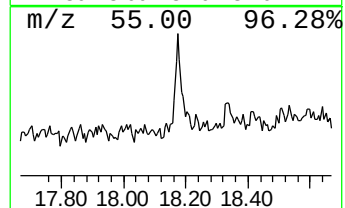
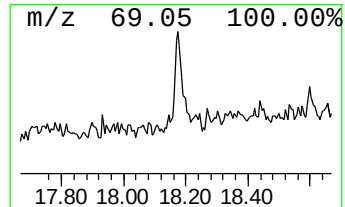
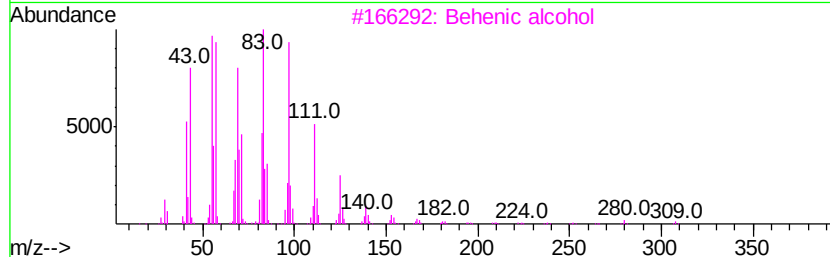
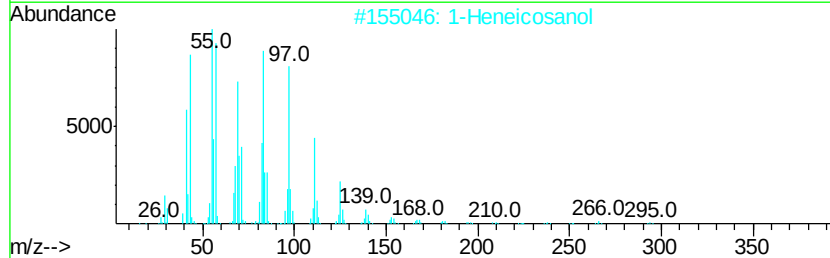
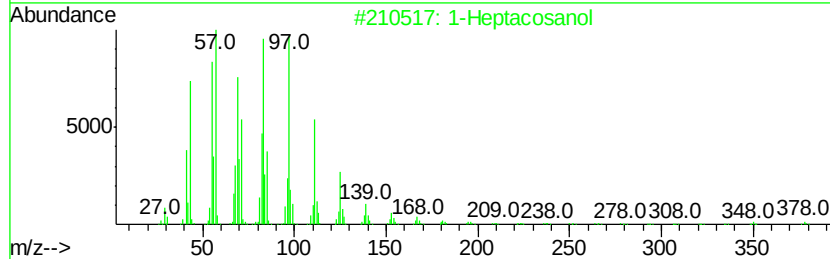
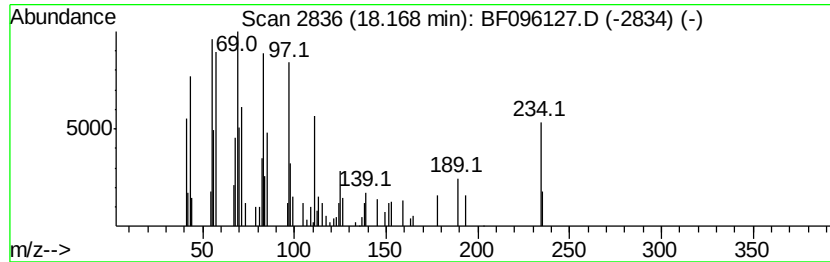
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ClientSampleId :
GHD-SB-020304-0-11

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Heptacosanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.17	2.77 ng	79381	Chrysene-d12	18.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	81
2	1-Heneicosanol	312	C21H44O	015594-90-8	81
3	Behenic alcohol	326	C22H46O	000661-19-8	81
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	70
5	Triacetyl acetate	480	C32H64O2	041755-58-2	64



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF062217\
Data File : BF096127.D
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Operator : SJ/MA
Sample : I3775-02
Misc :
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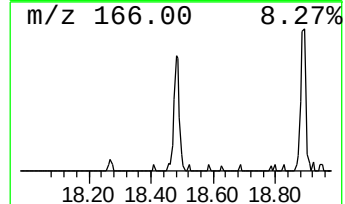
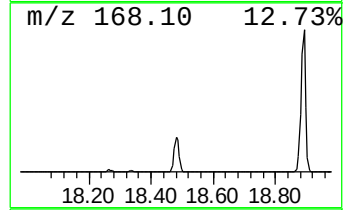
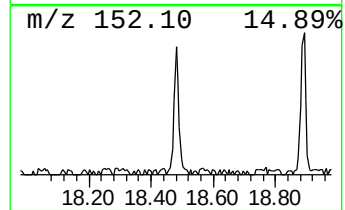
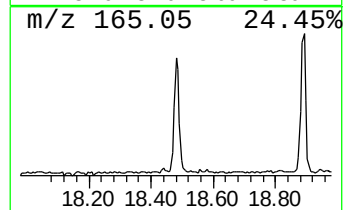
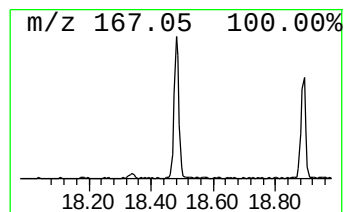
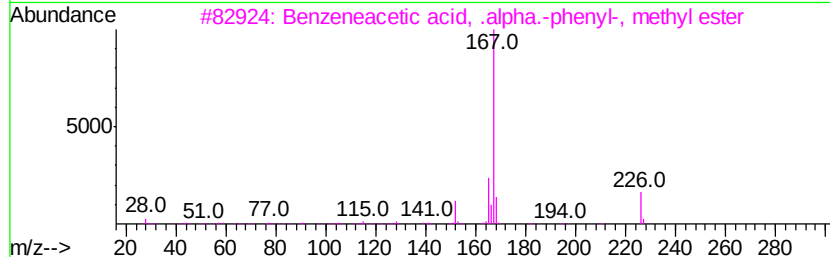
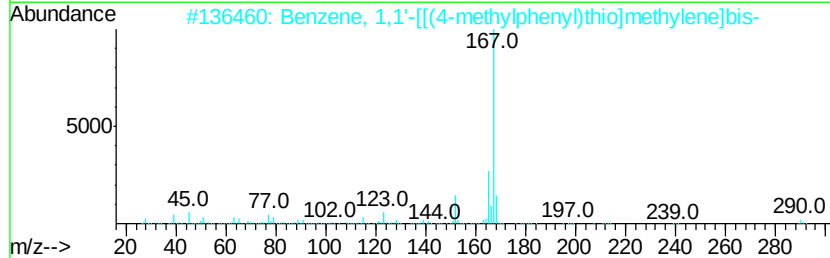
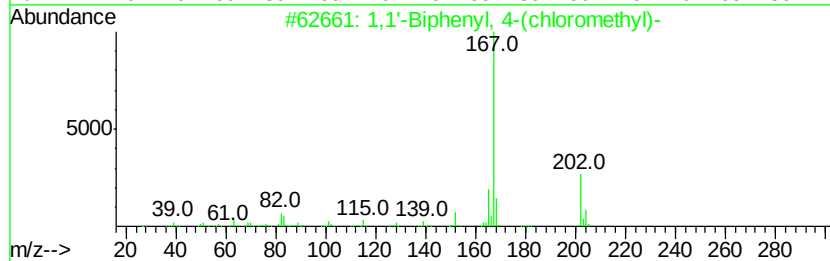
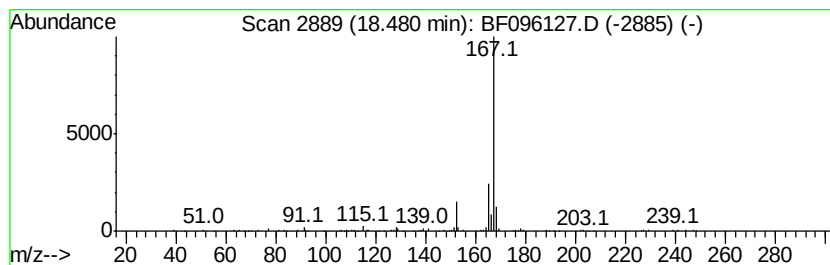
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,1'-Biphenyl, 4-(chloromet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.48	7.77 ng	222893	Chrysene-d12	18.27		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,1'-Biphenyl, 4-(chloromethyl)-	202	C13H11Cl	001667-11-4	86
2		Benzene, 1,1'-[[(4-methylphenyl)...	290	C20H18S	032110-49-9	78
3		Benzeneacetic acid, .alpha.-phen...	226	C15H14O2	003469-00-9	78
4		2-Propanone, 1,1-diphenyl-	210	C15H14O	000781-35-1	78
5		1-Benzhydrylazetidin-3-ol	239	C16H17NO	018621-17-5	78



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF062217\
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Acq On : 22 Jun 2017 17:54
Operator : SJ/MA
Sample : I3775-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

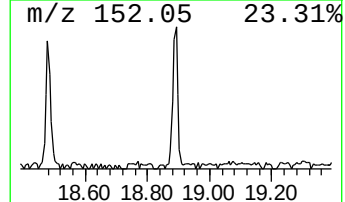
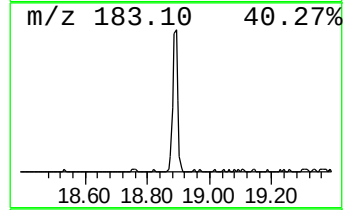
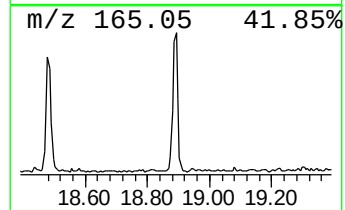
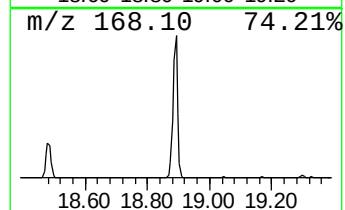
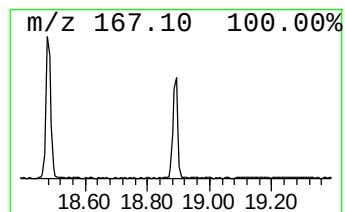
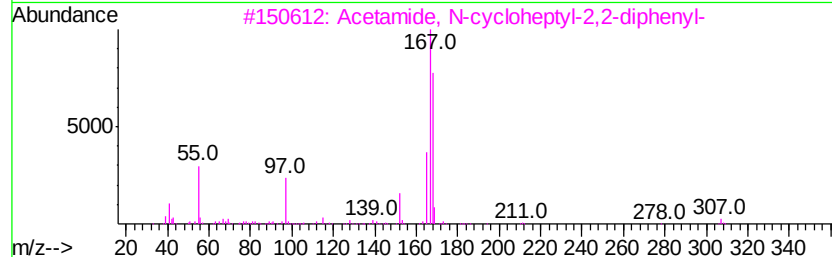
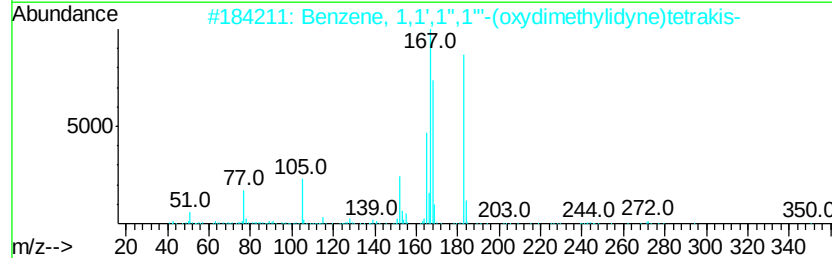
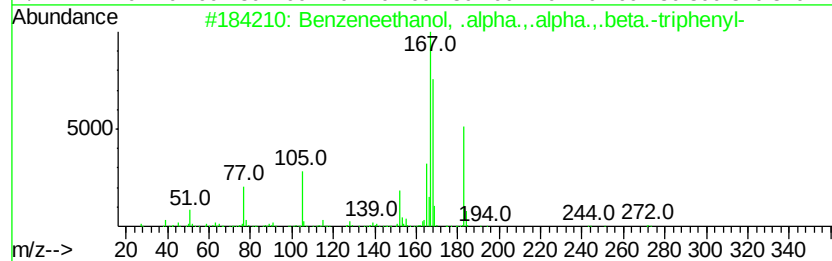
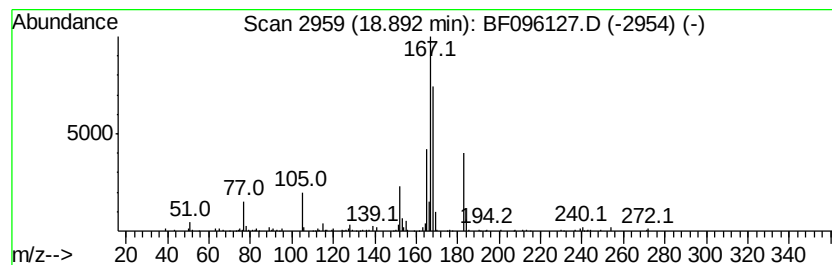
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Benzeneethanol, .alpha.,.al... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.89	8.20 ng	235262	Chrysene-d12	18.27		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzeneethanol, .alpha.,.alpha.,...	350	C26H22O	000981-24-8	90
2		Benzene, 1,1',1'',1'''-(oxydimet...	350	C26H22O	000574-42-5	80
3		Acetamide, N-cvcloheptyl-2,2-dip...	307	C21H25NO	351062-01-6	58
4		1,2-Diphenylethyl isothiocyanate	239	C15H13NS	1000134-54-2	50
5		Diphenylmethane	168	C13H12	000101-81-5	49



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF062217\
Data File : BF096127.D
Acq On : 22 Jun 2017 17:54
Operator : SJ/MA
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GHD-SB-020304-0-11

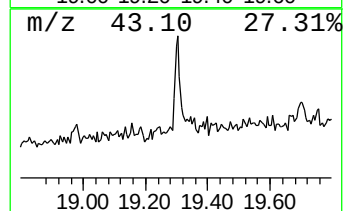
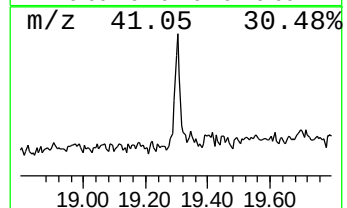
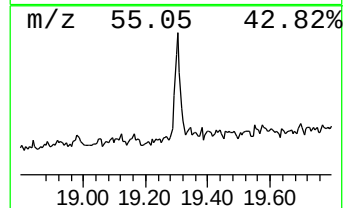
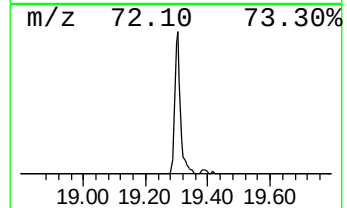
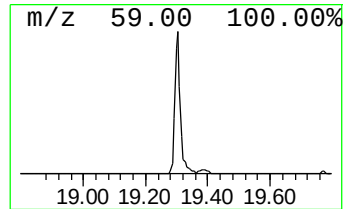
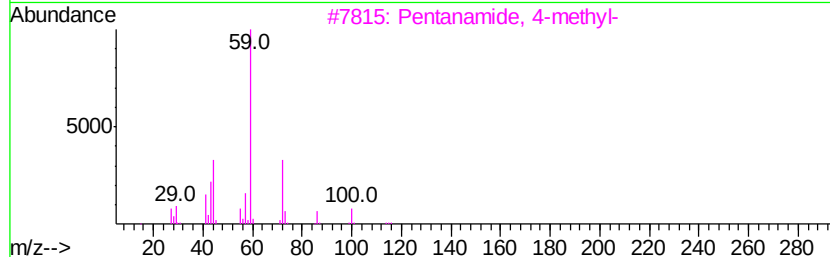
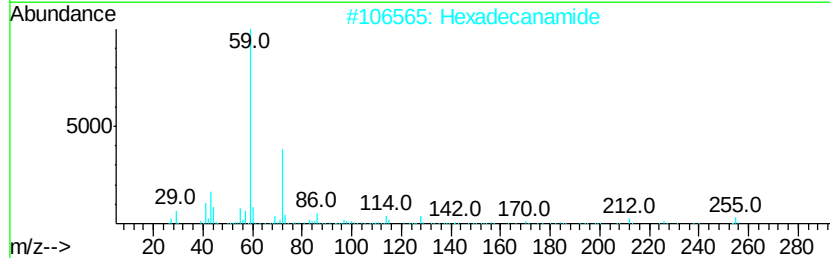
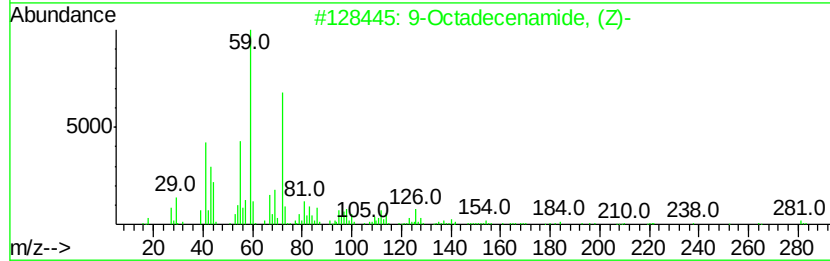
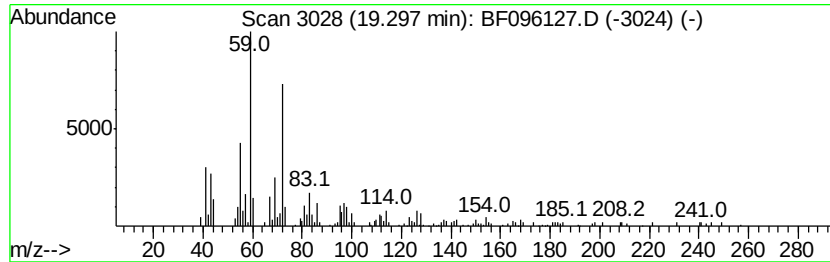
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.30	10.32 ng	191971	Perylene-d12	19.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2		Hexadecanamide	255	C16H33NO	000629-54-9	53
3		Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
4		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	47
5		Dodecanamide	199	C12H25NO	001120-16-7	47



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF062217\
Data File : BF096127.D
Acq On : 22 Jun 2017 17:54
Operator : SJ/MA
Sample : I3775-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHD-SB-020304-0-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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...	4.45	12.9	ng	254066	1	7.27	394496	20.0
unknown6.94	6.94	96.0	ng	1893160	1	7.27	394496	20.0
Hexadecane	13.76	2.3	ng	52929	4	14.53	460992	20.0
n-Hexadecanoic acid	15.56	2.6	ng	60647	4	14.53	460992	20.0
unknown18.04	18.04	2.3	ng	65132	5	18.27	573904	20.0
1-Heptacosanol	18.17	2.8	ng	79381	5	18.27	573904	20.0
1,1'-Biphenyl, 4-...	18.48	7.8	ng	222893	5	18.27	573904	20.0
Benzeneethanol, ...	18.89	8.2	ng	235262	5	18.27	573904	20.0
9-Octadecenamide, ...	19.30	10.3	ng	191971	6	19.94	372126	20.0