

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062417\
 Data File : BF096189.D
 Acq On : 24 Jun 2017 14:32
 Operator : SJ/MA
 Sample : I3851-09
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 G-37-0-1.5

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	1.540	7	9	31	rBV	568270	1028460	62.49%	7.228%
2	4.410	493	497	517	rBV	58857	179497	10.91%	1.261%
3	5.140	617	621	651	rBV	468963	1240344	75.37%	8.717%
4	6.839	906	910	920	rBV	569572	1089873	66.22%	7.659%
5	6.922	920	924	947	rVB	878103	1645751	100.00%	11.566%
6	7.257	978	981	995	rBV	252897	368297	22.38%	2.588%
7	7.498	1017	1022	1044	rBV	759825	1078913	65.56%	7.582%
8	8.186	1134	1139	1157	rBV	443782	775770	47.14%	5.452%
9	9.292	1323	1327	1341	rBV	305189	482788	29.34%	3.393%
10	11.075	1625	1630	1650	rBV	1215565	1512598	91.91%	10.630%
11	11.774	1745	1749	1761	rBV	119813	166492	10.12%	1.170%
12	12.116	1802	1807	1812	rBV2	358813	451202	27.42%	3.171%
13	12.163	1812	1815	1821	rVB2	26658	34442	2.09%	0.242%
14	12.974	1946	1953	1957	rVB2	24694	31094	1.89%	0.219%
15	13.416	2024	2028	2043	rBV	377604	606173	36.83%	4.260%
16	13.704	2070	2077	2081	rBV	26718	58596	3.56%	0.412%
17	13.745	2081	2084	2092	rVB2	30340	56250	3.42%	0.395%
18	14.427	2195	2200	2204	rBV3	27253	35591	2.16%	0.250%
19	14.474	2204	2208	2210	rVV2	19002	21217	1.29%	0.149%
20	14.510	2210	2214	2219	rVV	296773	392126	23.83%	2.756%
21	14.551	2219	2221	2229	rVB2	38320	55458	3.37%	0.390%
22	14.651	2235	2238	2245	rBV2	11953	20163	1.23%	0.142%
23	15.333	2348	2354	2358	rBV5	10706	19914	1.21%	0.140%
24	15.539	2385	2389	2396	rVB3	49809	72806	4.42%	0.512%
25	15.774	2425	2429	2437	rVB6	14297	25931	1.58%	0.182%
26	16.139	2488	2491	2495	rBV2	12177	17065	1.04%	0.120%
27	16.345	2520	2526	2533	rBV	104914	133638	8.12%	0.939%
28	16.651	2574	2578	2584	rBV	166858	217554	13.22%	1.529%
29	16.898	2615	2620	2630	rBV	956244	1088696	66.15%	7.651%
30	17.092	2649	2653	2654	rBV4	18706	21071	1.28%	0.148%
31	17.262	2678	2682	2687	rBV4	23442	45352	2.76%	0.319%
32	17.380	2698	2702	2705	rBV3	11243	20309	1.23%	0.143%
33	17.568	2731	2734	2737	rBV3	24499	28181	1.71%	0.198%
34	18.162	2831	2835	2841	rBV3	78911	135165	8.21%	0.950%

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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	18.250	2845	2850	2855	rBV2	371995	508700	30.91%	3.575%
36	18.321	2860	2862	2865	rVB	55005	56967	3.46%	0.400%
37	19.292	3024	3027	3031	rVB2	100498	114699	6.97%	0.806%
38	19.527	3065	3067	3072	rBV2	67071	89850	5.46%	0.631%
39	19.933	3132	3136	3143	rBV	239390	302211	18.36%	2.124%

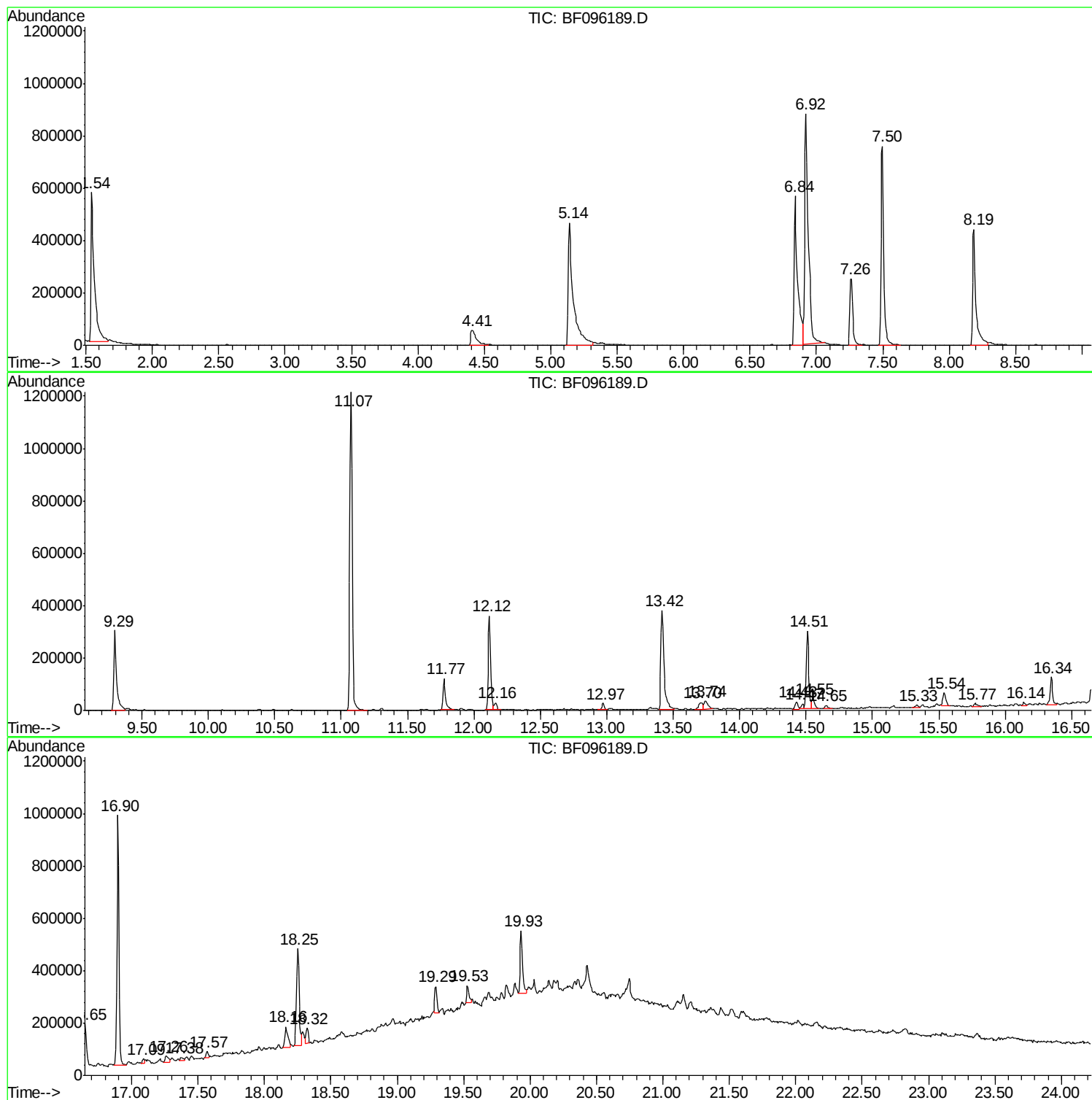
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ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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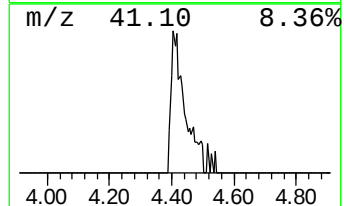
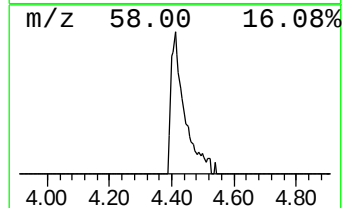
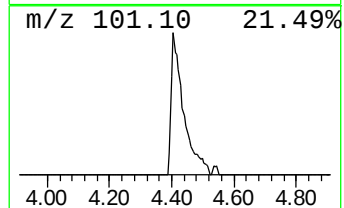
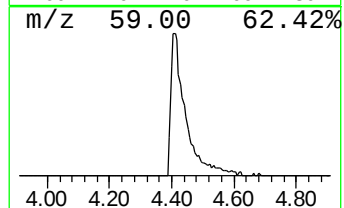
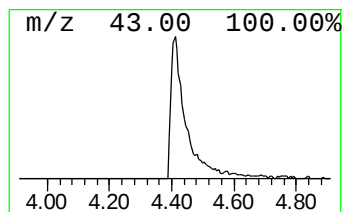
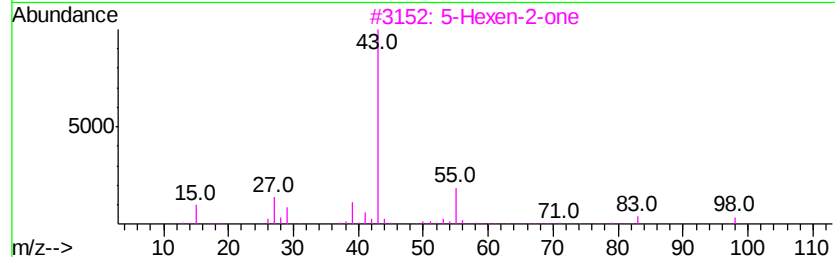
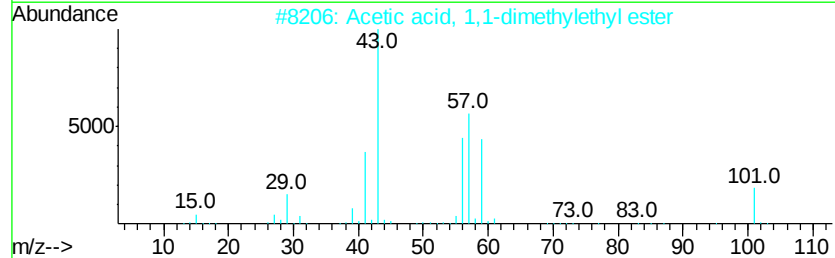
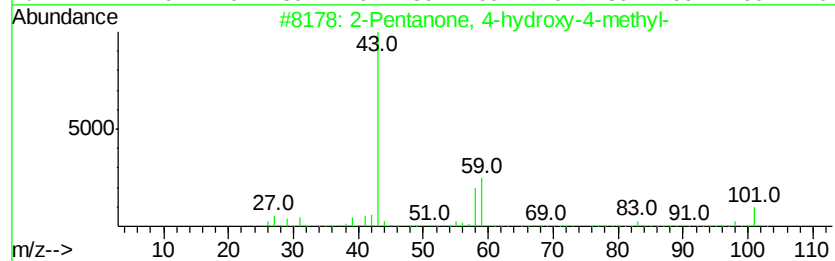
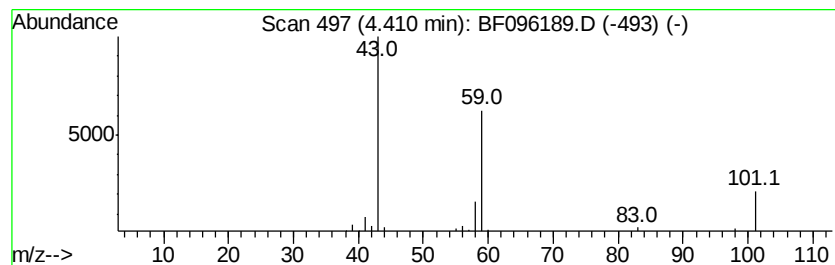
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	9.75 ng	179497	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	40
3		5-Hexen-2-one	98	C6H10O	000109-49-9	10
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Guanidine	59	CH5N3	000113-00-8	9



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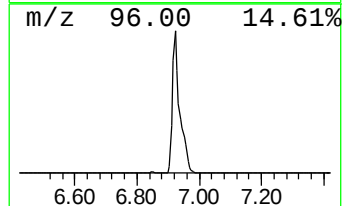
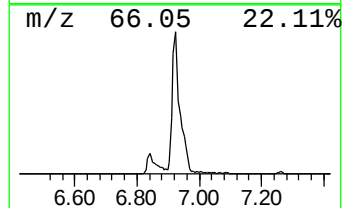
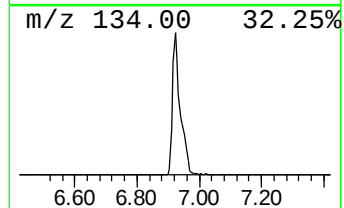
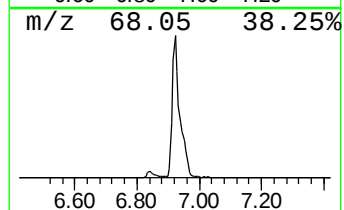
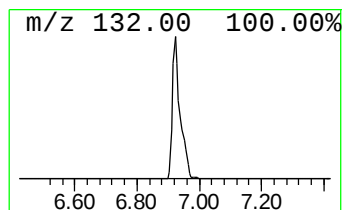
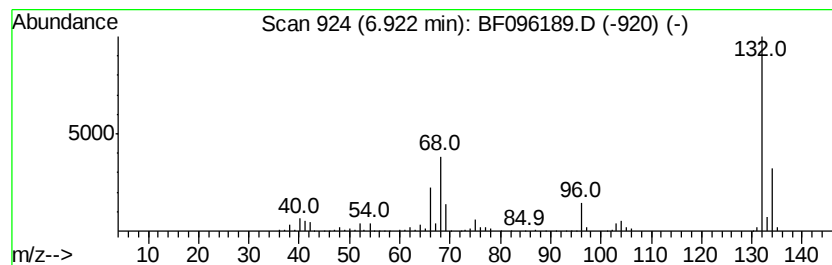
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.92 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.92	89.37 ng	1645750	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	30
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Indazole, 7-methyl-	132	C8H8N2	1000316-00-7	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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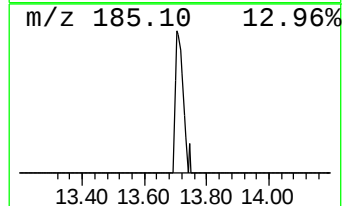
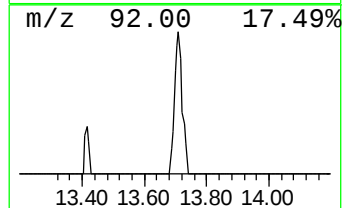
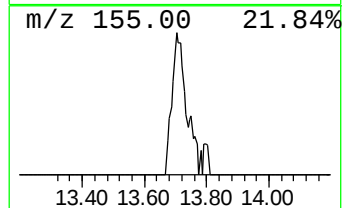
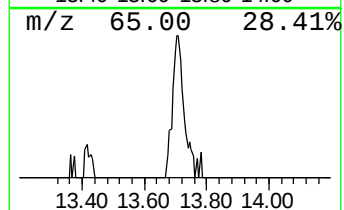
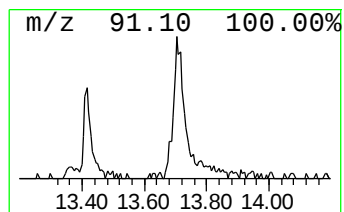
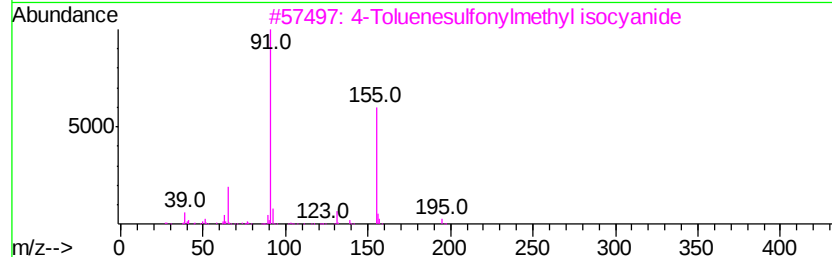
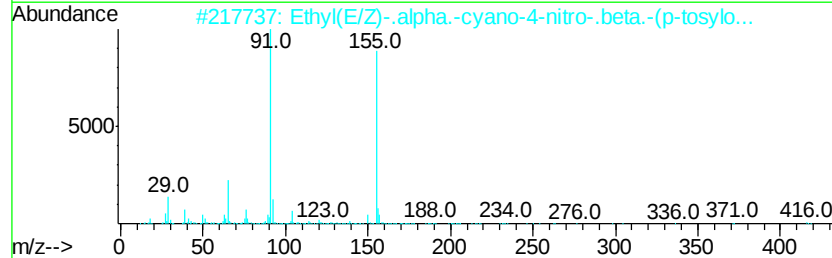
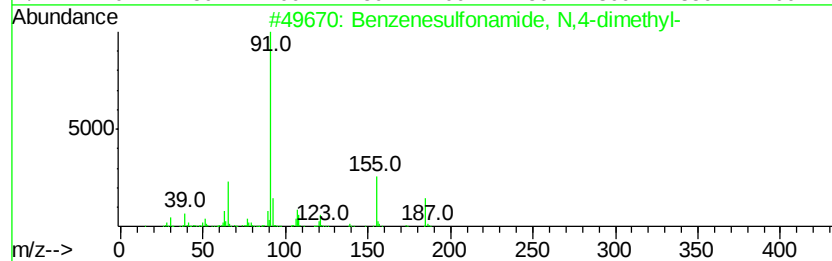
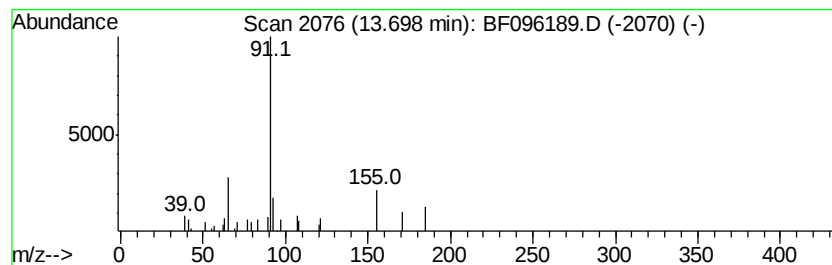
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Benzenesulfonamide, N,4-dim... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.99 ng	58596	Phenanthrene-d10	14.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	90
2		Ethyl(E/Z)-.alpha.-cyano-4-nitro...	416	C19H16N2O7S	1000287-26-8	47
3		4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	47
4		Benzenemethanesulfonamide	171	C7H9NO2S	004563-33-1	47
5		Tricyclo[2.1.1.0(5,6)]hexane-2-c...	275	C14H13NO3S	103495-50-7	42



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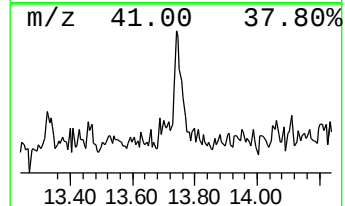
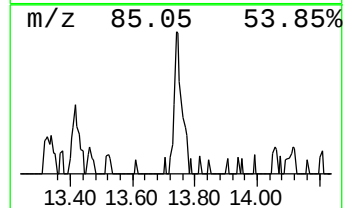
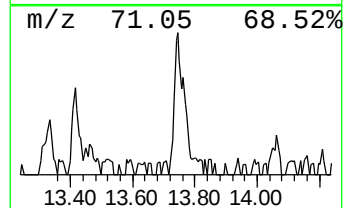
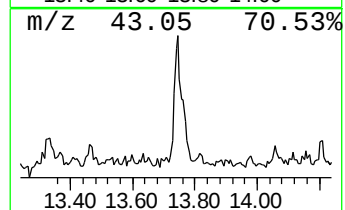
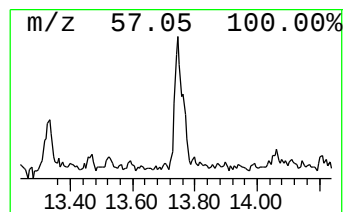
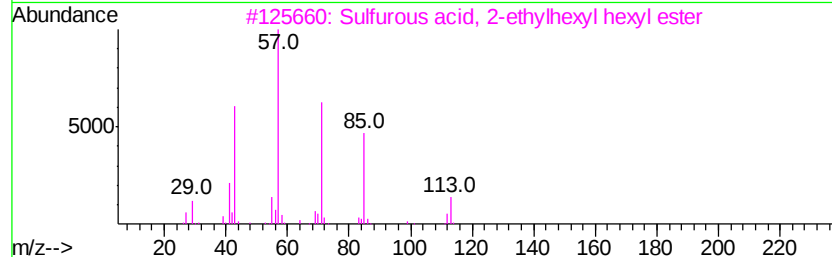
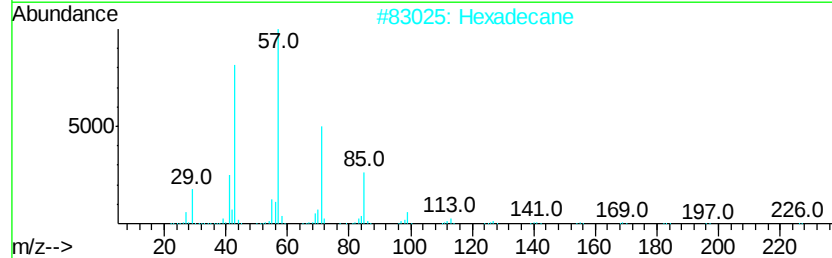
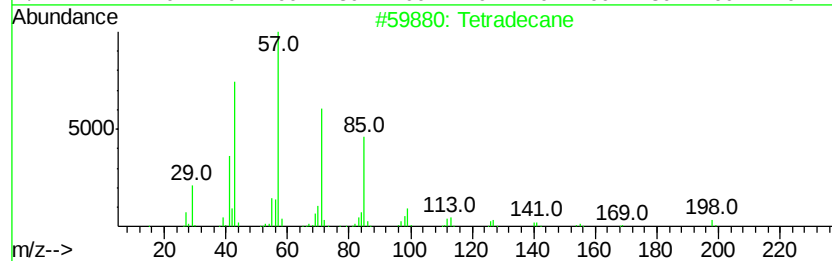
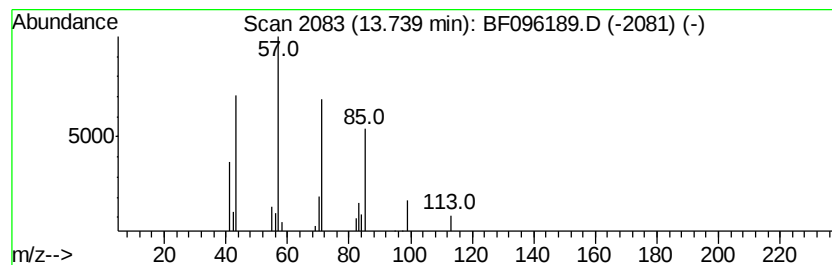
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Tetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.74	2.87 ng	56250	Phenanthrene-d10	14.51	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	72
2	Hexadecane	226	C16H34	000544-76-3	72
3	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64
4	Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	59
5	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	59



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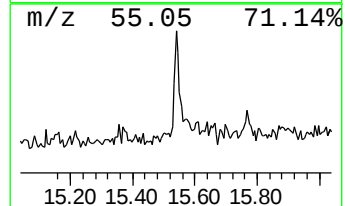
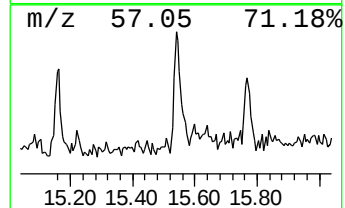
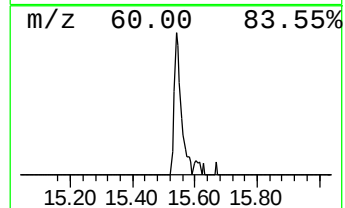
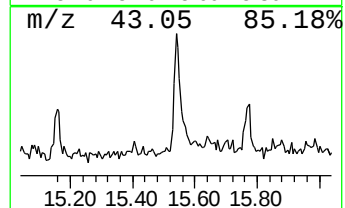
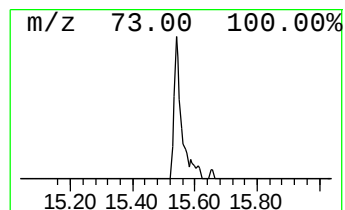
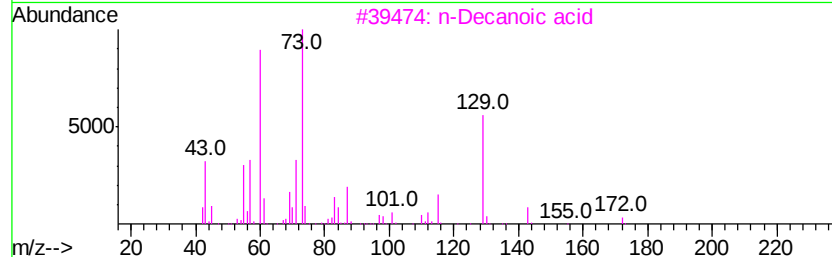
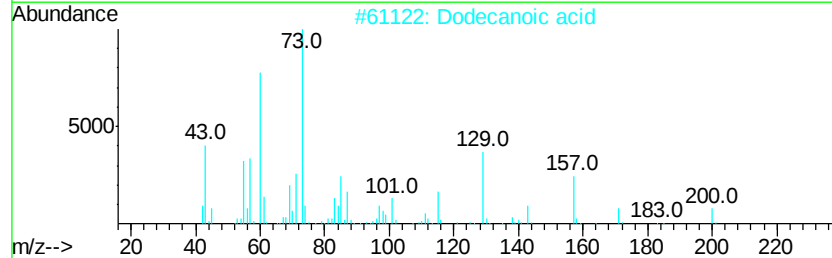
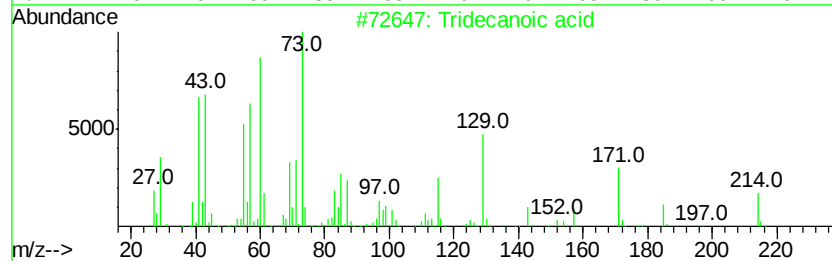
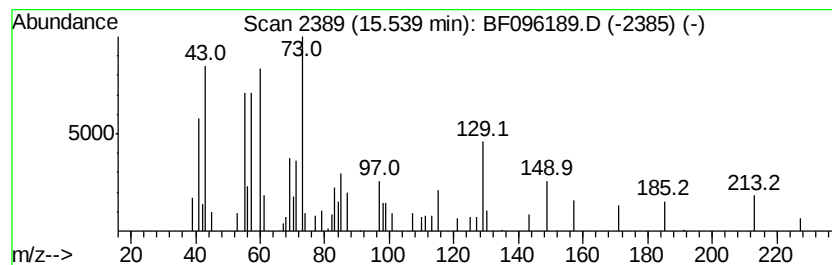
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Tridecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	3.71 ng	72806	Phenanthrene-d10	14.51

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	74
2		Dodecanoic acid	200	C12H24O2	000143-07-7	64
3		n-Decanoic acid	172	C10H20O2	000334-48-5	50
4		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38
5		Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	38



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Misc :
ALS Vial : 11 Sample Multiplier: 1

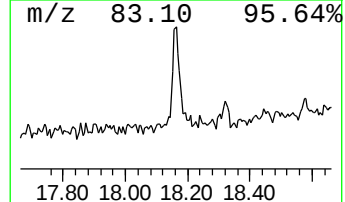
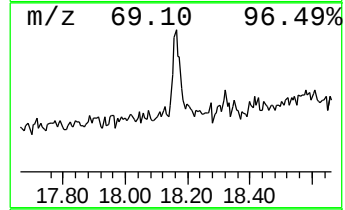
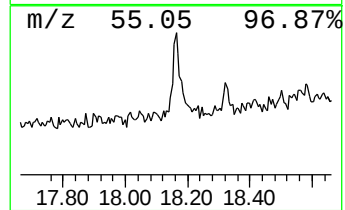
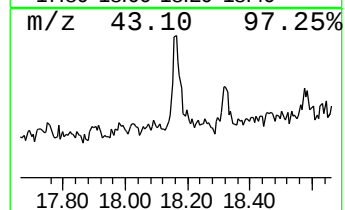
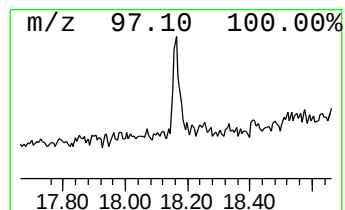
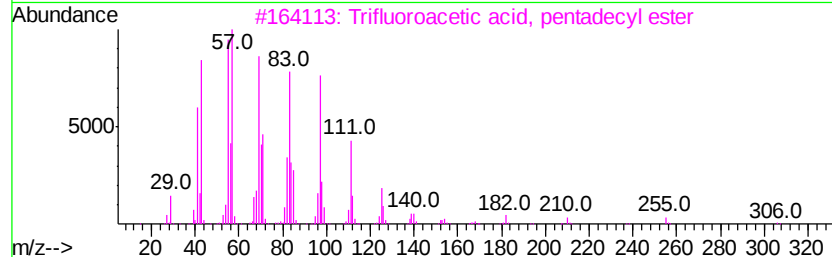
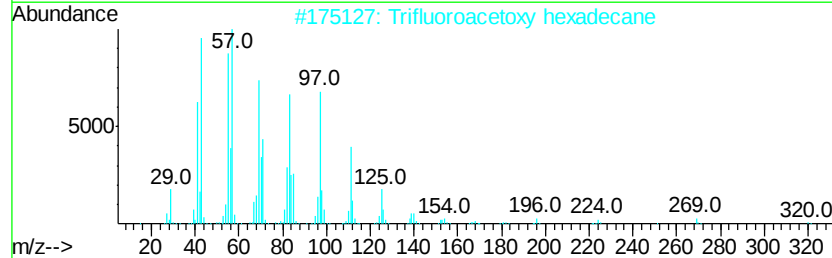
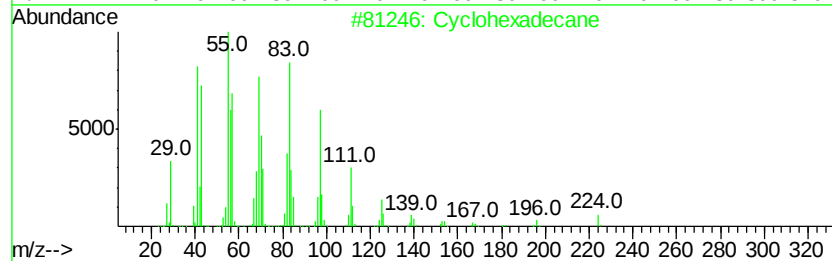
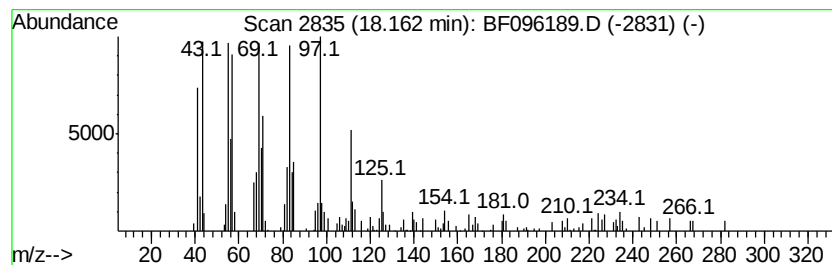
Instrument :
BNA_F
ClientSampleId :
G-37-0-1.5

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 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.16	5.31 ng	135165	Chrysene-d12	18.25
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Cyclohexadecane	224 C16H32	000295-65-8 95
2		Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3 94
3		Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2 93
4		Trichloroacetic acid, hexadecyl ...	386 C18H33Cl3O2	074339-54-1 91
5		Carbonic acid, octadecyl 2,2,2-t...	444 C21H39Cl3O3	1000314-56-3 91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062417\
Data File : BF096189.D
Acq On : 24 Jun 2017 14:32
Operator : SJ/MA
Sample : I3851-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-37-0-1.5

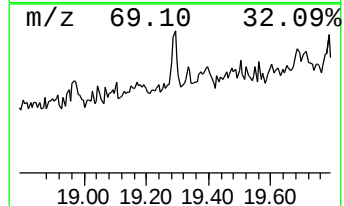
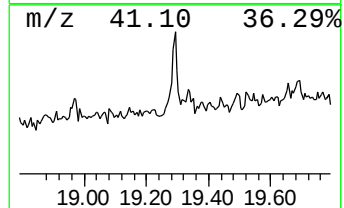
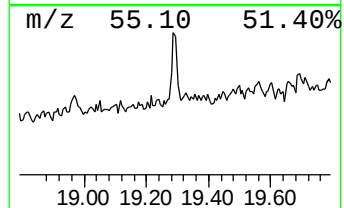
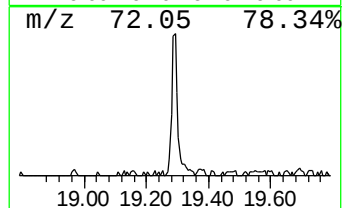
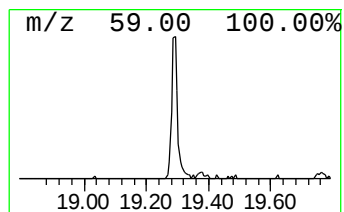
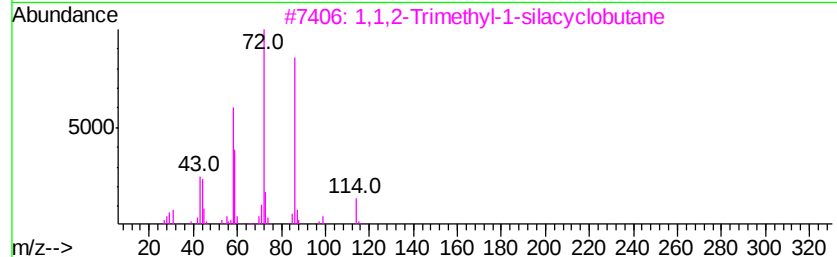
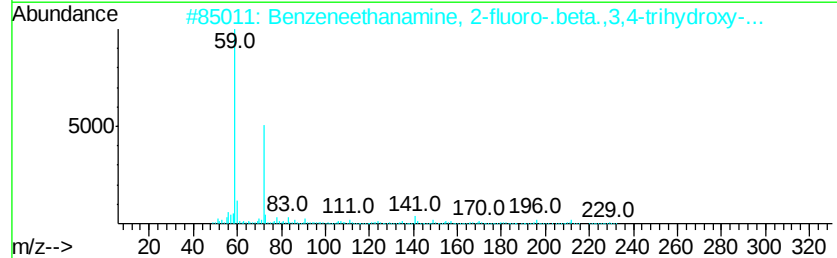
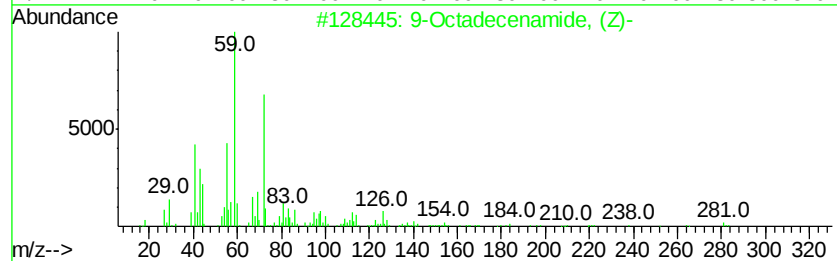
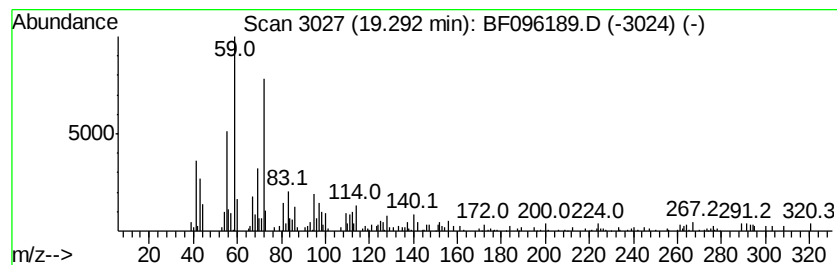
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.29	7.59 ng	114699	Perylene-d12	19.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	80
2		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
3		1,1,2-Trimethyl-1-silacyclobutane	114	C6H14Si	030681-90-4	43
4		Octadecanamide	283	C18H37NO	000124-26-5	38
5		Decanamide-	171	C10H21NO	002319-29-1	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062417\
Data File : BF096189.D
Acq On : 24 Jun 2017 14:32
Operator : SJ/MA
Sample : I3851-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
G-37-0-1.5

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...	4.41	9.8	ng	179497	1	7.26	368297	20.0
unknown6.92	6.92	89.4	ng	1645750	1	7.26	368297	20.0
Benzenesulfonamid...	13.70	3.0	ng	58596	4	14.51	392126	20.0
Tetradecane	13.74	2.9	ng	56250	4	14.51	392126	20.0
Tridecanoic acid	15.54	3.7	ng	72806	4	14.51	392126	20.0
Cyclohexadecane	18.16	5.3	ng	135165	5	18.25	508700	20.0
9-Octadecenamide, ...	19.29	7.6	ng	114699	6	19.93	302211	20.0