

Data Path : Z:\HPCHEM1\BNA F\DATA\BF060217\
 Data File : BF095637.D
 Acq On : 2 Jun 2017 16:52
 Operator : SJ/MA
 Sample : I3412-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-3-TP-4-COMP

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-BF050217.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	4.804	526	530	551	rBV2	69230	212052	7.33%	0.885%
2	5.451	636	640	672	rBV	1233337	2479395	85.67%	10.344%
3	7.086	914	918	932	rBV	1456724	2484340	85.84%	10.365%
4	7.192	932	936	956	rVB	1817322	2893989	100.00%	12.074%
5	7.539	990	995	1009	rVB	438851	636203	21.98%	2.654%
6	7.775	1030	1035	1057	rBV	1332589	1947570	67.30%	8.126%
7	8.451	1145	1150	1186	rBV	971758	1586052	54.81%	6.617%
8	9.569	1336	1340	1361	rBV	512863	773450	26.73%	3.227%
9	11.345	1636	1642	1657	rBV	2001744	2540025	87.77%	10.597%
10	11.633	1686	1691	1697	rVB2	28740	39555	1.37%	0.165%
11	12.045	1757	1761	1772	rBV	131839	202334	6.99%	0.844%
12	12.392	1815	1820	1834	rBV2	708484	941190	32.52%	3.927%
13	13.239	1959	1964	1968	rBV	28537	36362	1.26%	0.152%
14	13.692	2036	2041	2056	rBV	924506	1490421	51.50%	6.218%
15	14.009	2086	2095	2105	rBV	39653	65734	2.27%	0.274%
16	14.739	2214	2219	2224	rBV	30723	41829	1.45%	0.175%
17	14.798	2224	2229	2248	rVB	603539	965215	33.35%	4.027%
18	15.780	2389	2396	2405	rBV4	57931	98873	3.42%	0.413%
19	16.562	2526	2529	2533	rBV2	27745	30767	1.06%	0.128%
20	16.615	2534	2538	2548	rVB	56737	77685	2.68%	0.324%
21	16.880	2579	2583	2586	rBV	40732	55949	1.93%	0.233%
22	16.921	2586	2590	2598	rVB	60835	94354	3.26%	0.394%
23	17.145	2623	2628	2637	rVB	1881649	2157458	74.55%	9.001%
24	18.386	2835	2839	2852	rBV4	69822	138388	4.78%	0.577%
25	18.492	2853	2857	2876	rVB	507993	789935	27.30%	3.296%
26	19.186	2970	2975	2983	rBV10	13413	31016	1.07%	0.129%
27	19.515	3027	3031	3043	rBV	267226	351735	12.15%	1.467%
28	19.786	3074	3077	3081	rBV	27846	32248	1.11%	0.135%
29	20.127	3131	3135	3138	rBV	30313	43060	1.49%	0.180%
30	20.168	3138	3142	3153	rVV	404381	626197	21.64%	2.613%
31	20.250	3153	3156	3162	rVB7	17361	31964	1.10%	0.133%
32	20.597	3211	3215	3219	rBV5	19234	31881	1.10%	0.133%
33	21.462	3358	3362	3367	rBV6	21318	41089	1.42%	0.171%

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Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3-TP-4-COMP

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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

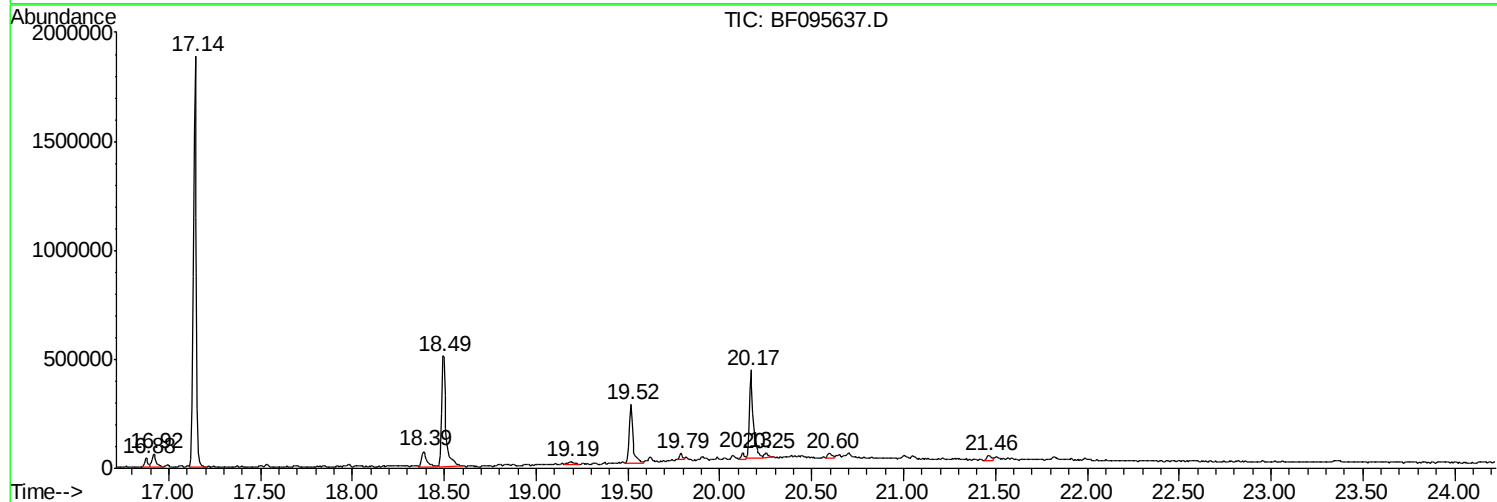
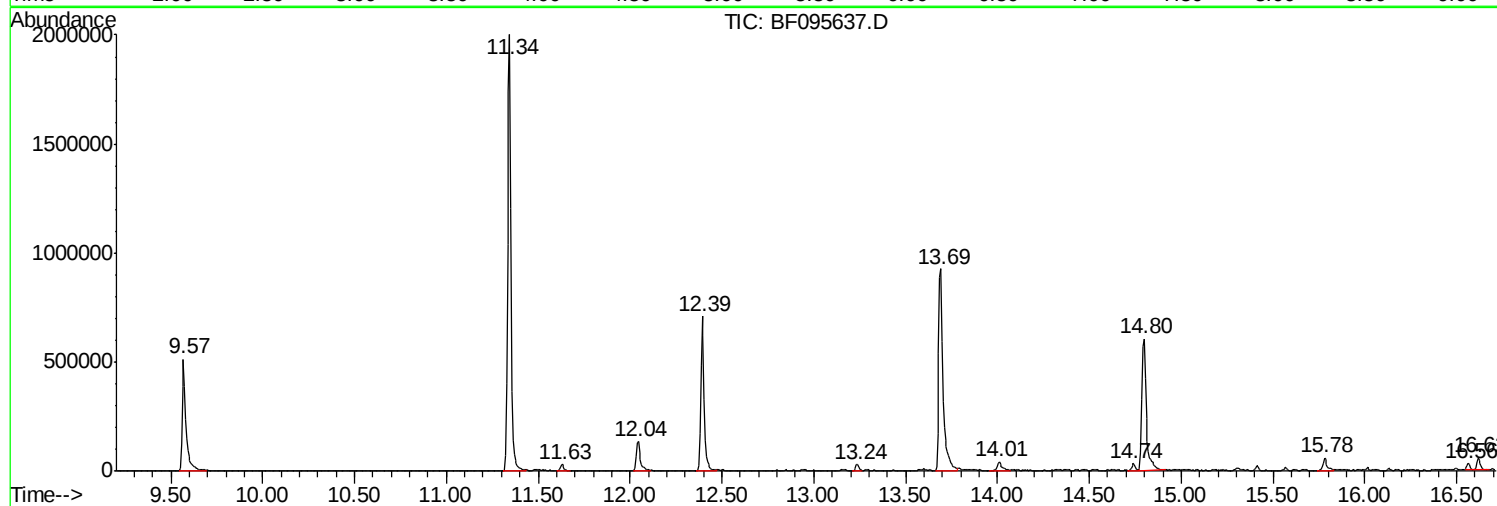
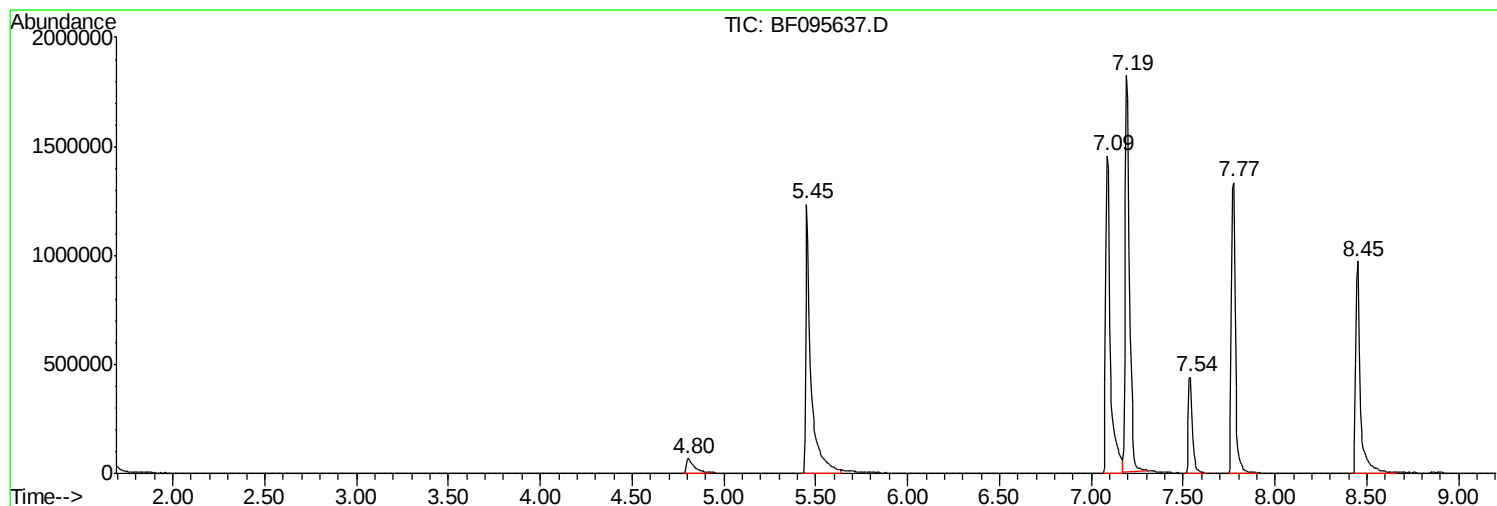
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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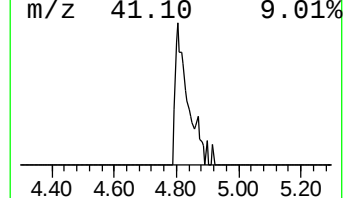
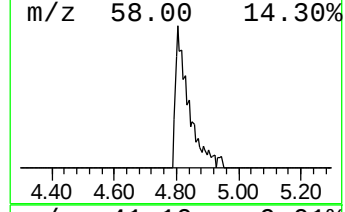
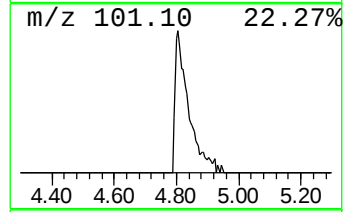
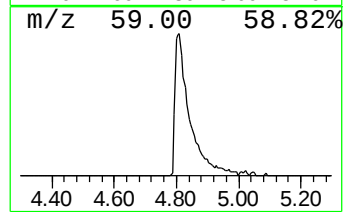
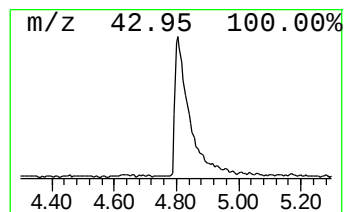
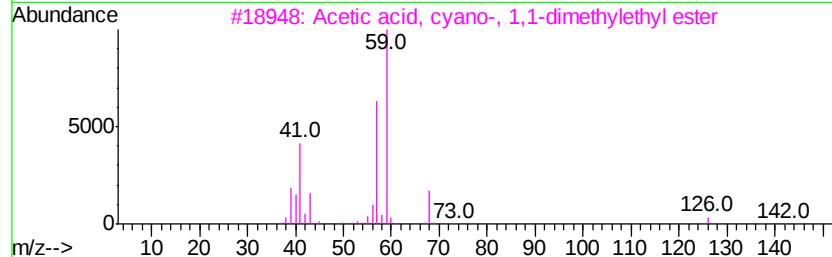
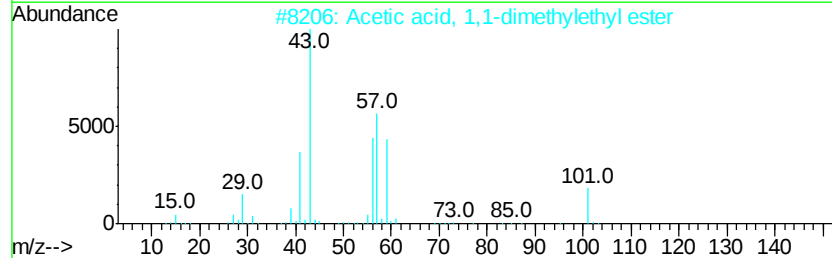
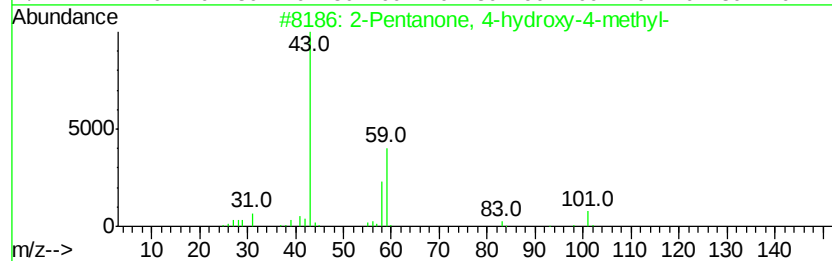
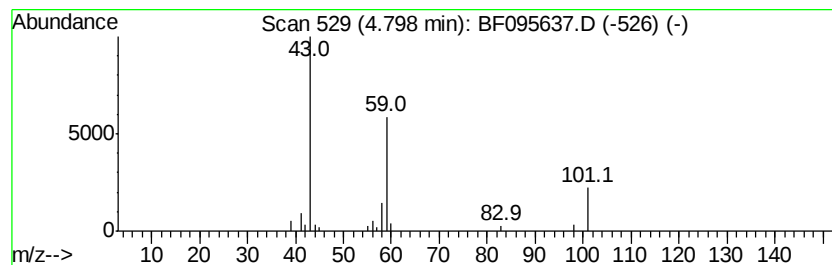
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	6.67 ng	212052	1,4-Dichlorobenzene-d4	7.54

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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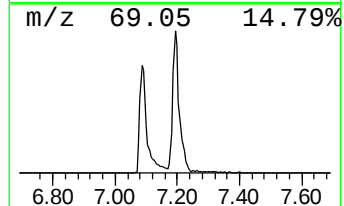
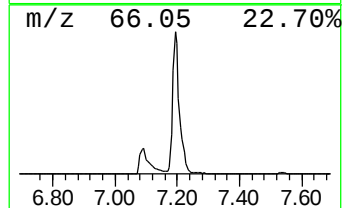
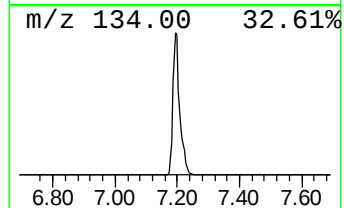
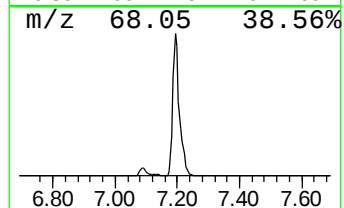
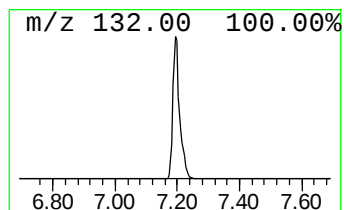
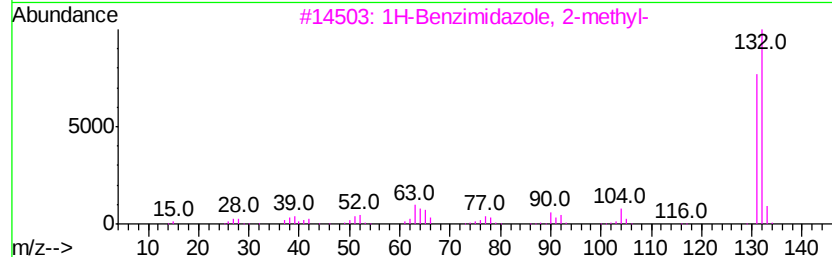
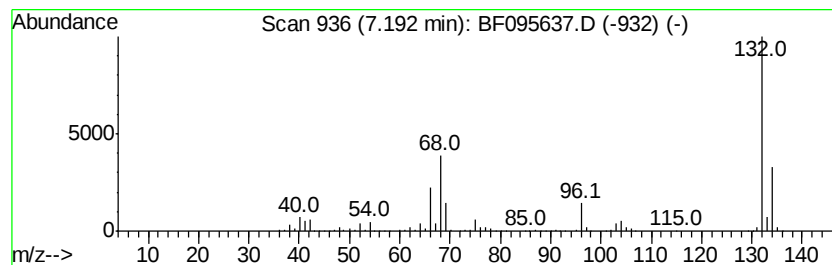
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.19 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	90.98 ng	2893990	1,4-Dichlorobenzene-d4	7.54

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		Xenon	132	Xe	007440-63-3	9



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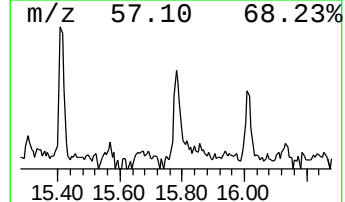
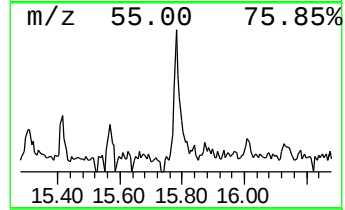
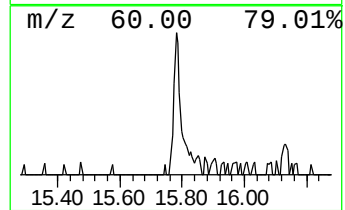
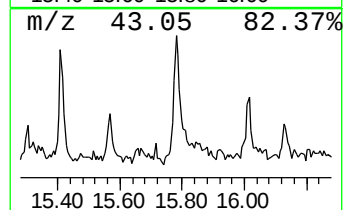
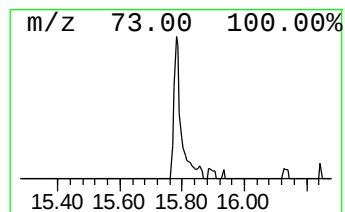
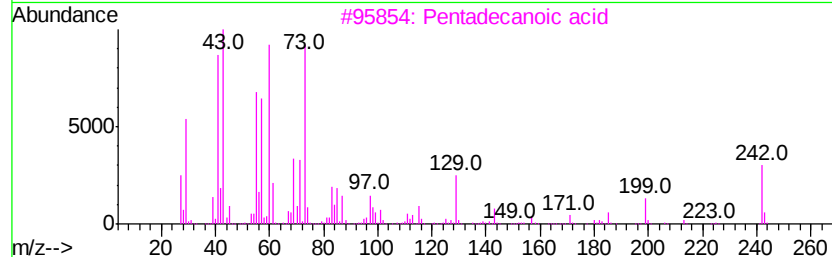
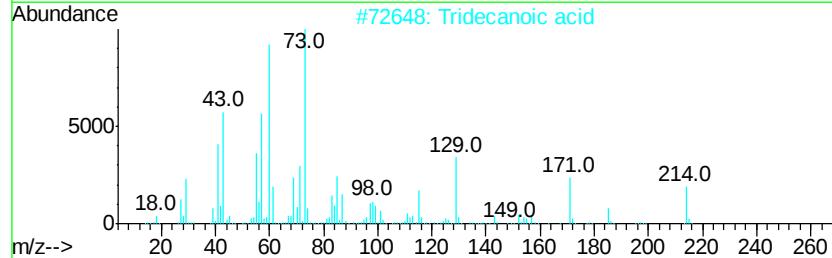
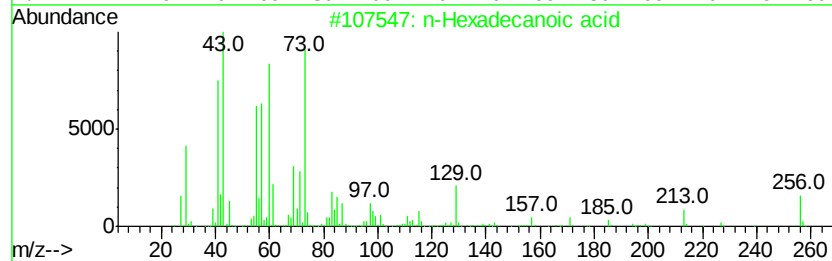
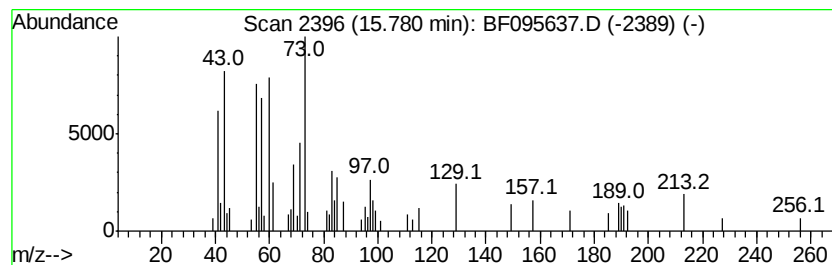
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.78	2.05 ng	98873	Phenanthrene-d10	14.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
2		Tridecanoic acid	214	C13H26O2	000638-53-9	50
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	50
4		n-Decanoic acid	172	C10H20O2	000334-48-5	47
5		Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	18



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Misc :
ALS Vial : 7 Sample Multiplier: 1

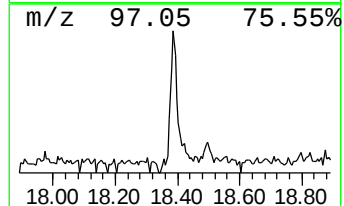
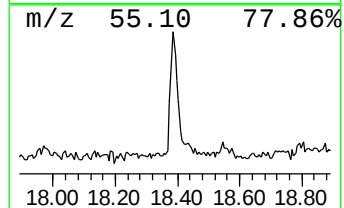
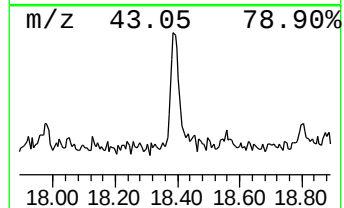
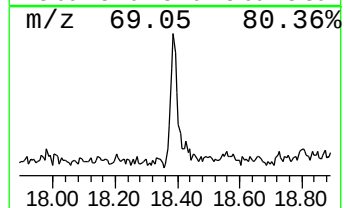
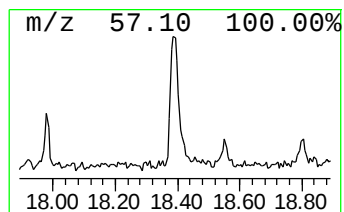
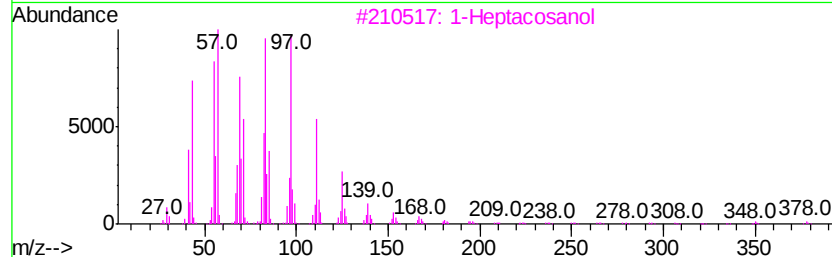
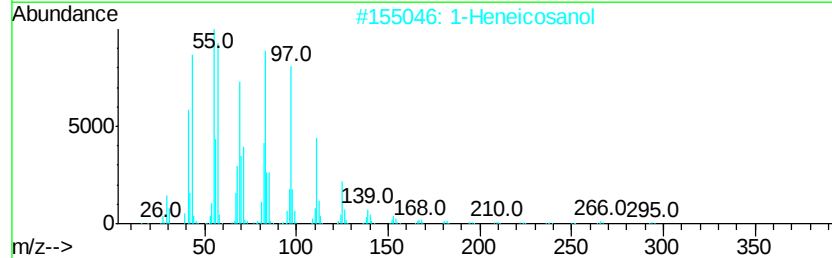
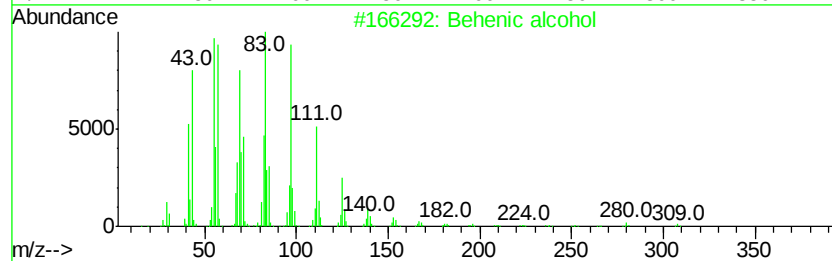
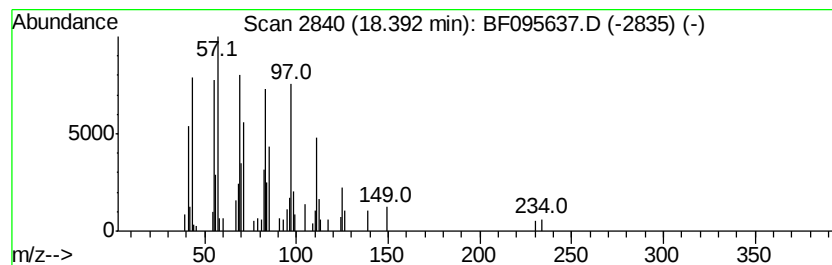
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.39	3.50 ng	138388	Chrysene-d12		18.50
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87



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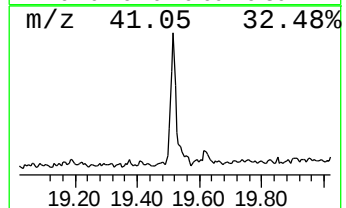
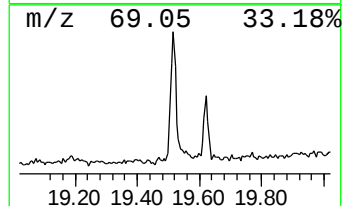
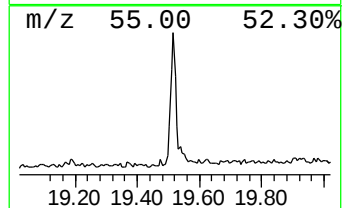
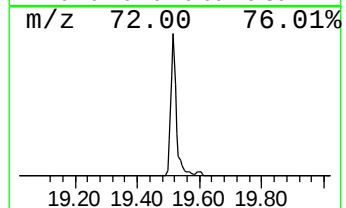
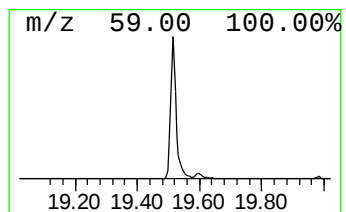
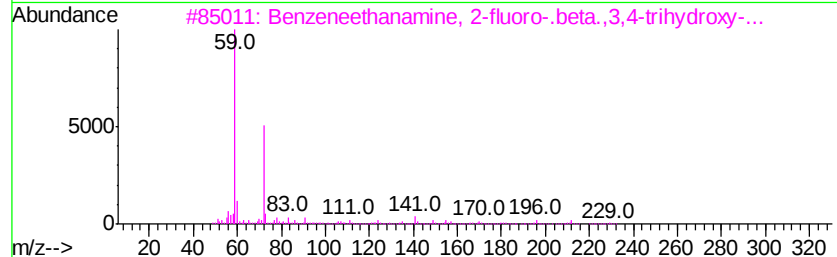
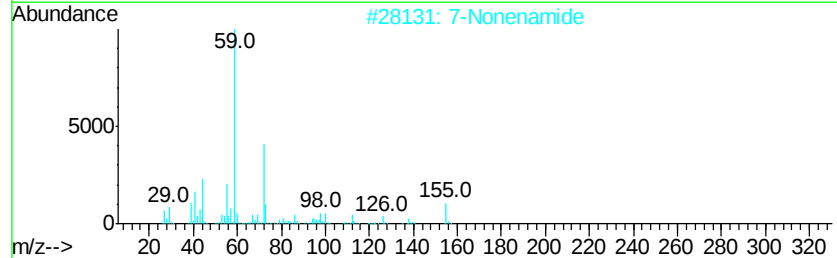
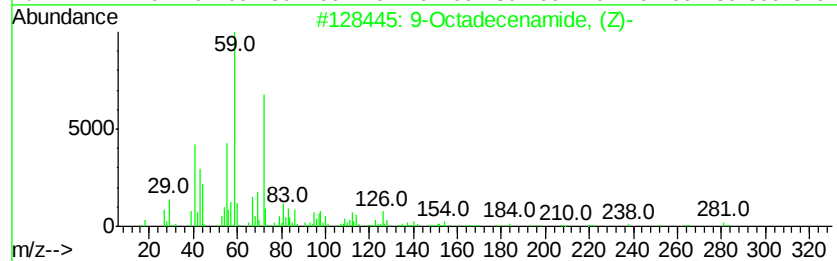
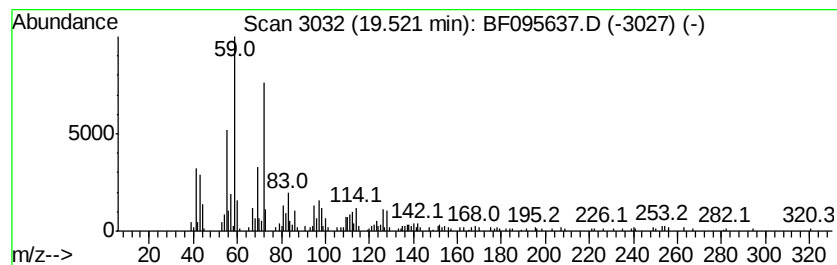
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.52	11.23 ng	351735	Perylene-d12	20.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2		7-Nonenamide	155	C9H17NO	090949-53-4	59
3		Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	53
4		Hexadecanamide	255	C16H33NO	000629-54-9	47
5		Dodecanamide	199	C12H25NO	001120-16-7	43



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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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...	4.80	6.7	ng	212052	1	7.54	636203	20.0
unknown7.19	7.19	91.0	ng	2893990	1	7.54	636203	20.0
n-Hexadecanoic acid	15.78	2.0	ng	98873	4	14.80	965215	20.0
Behenic alcohol	18.39	3.5	ng	138388	5	18.50	789935	20.0
9-Octadecenamide,...	19.52	11.2	ng	351735	6	20.17	626197	20.0