

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031219\  
 Data File : BG039883.D  
 Acq On : 12 Mar 2019 20:52  
 Operator : JU/SJ  
 Sample : K1842-04  
 Misc :  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 C-MW-10\_030719

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:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.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	3.205	15	20	29	rBV	176263	344709	8.60%	1.817%
2	3.281	29	33	45	rVB	176795	260742	6.51%	1.375%
3	5.696	438	444	454	rBV	438191	703880	17.57%	3.711%
4	7.294	710	716	725	rBV	298096	507668	12.67%	2.676%
5	7.681	774	782	795	rBV	759802	1300911	32.47%	6.858%
6	8.151	855	862	873	rVB	160247	273377	6.82%	1.441%
7	8.474	910	917	928	rVB	589760	1045917	26.10%	5.514%
8	9.332	1054	1063	1070	rBV	564399	1019342	25.44%	5.374%
9	9.496	1074	1091	1106	rBV	261249	958465	23.92%	5.053%
10	10.971	1334	1342	1351	rBV	212392	391774	9.78%	2.065%
11	11.788	1471	1481	1489	rBV4	14606	42854	1.07%	0.226%
12	13.403	1748	1756	1763	rBV	1575641	2430181	60.65%	12.811%
13	14.778	1983	1990	2000	rBV2	383614	613705	15.32%	3.235%
14	16.264	2236	2243	2258	rBV	1403737	2100060	52.41%	11.071%
15	17.521	2450	2457	2464	rBV2	555833	812428	20.28%	4.283%
16	20.117	2889	2899	2905	rBV	3013260	4006613	100.00%	21.122%
17	21.809	3179	3187	3200	rBV	566567	950284	23.72%	5.010%
18	23.290	3435	3439	3447	rVB2	24965	44722	1.12%	0.236%
19	23.495	3467	3474	3481	rVB	64134	118960	2.97%	0.627%
20	24.130	3575	3582	3588	rBV5	25651	55066	1.37%	0.290%
21	25.181	3741	3761	3778	rBV2	293279	941870	23.51%	4.965%
22	26.291	3942	3950	3960	rVB7	15197	45748	1.14%	0.241%

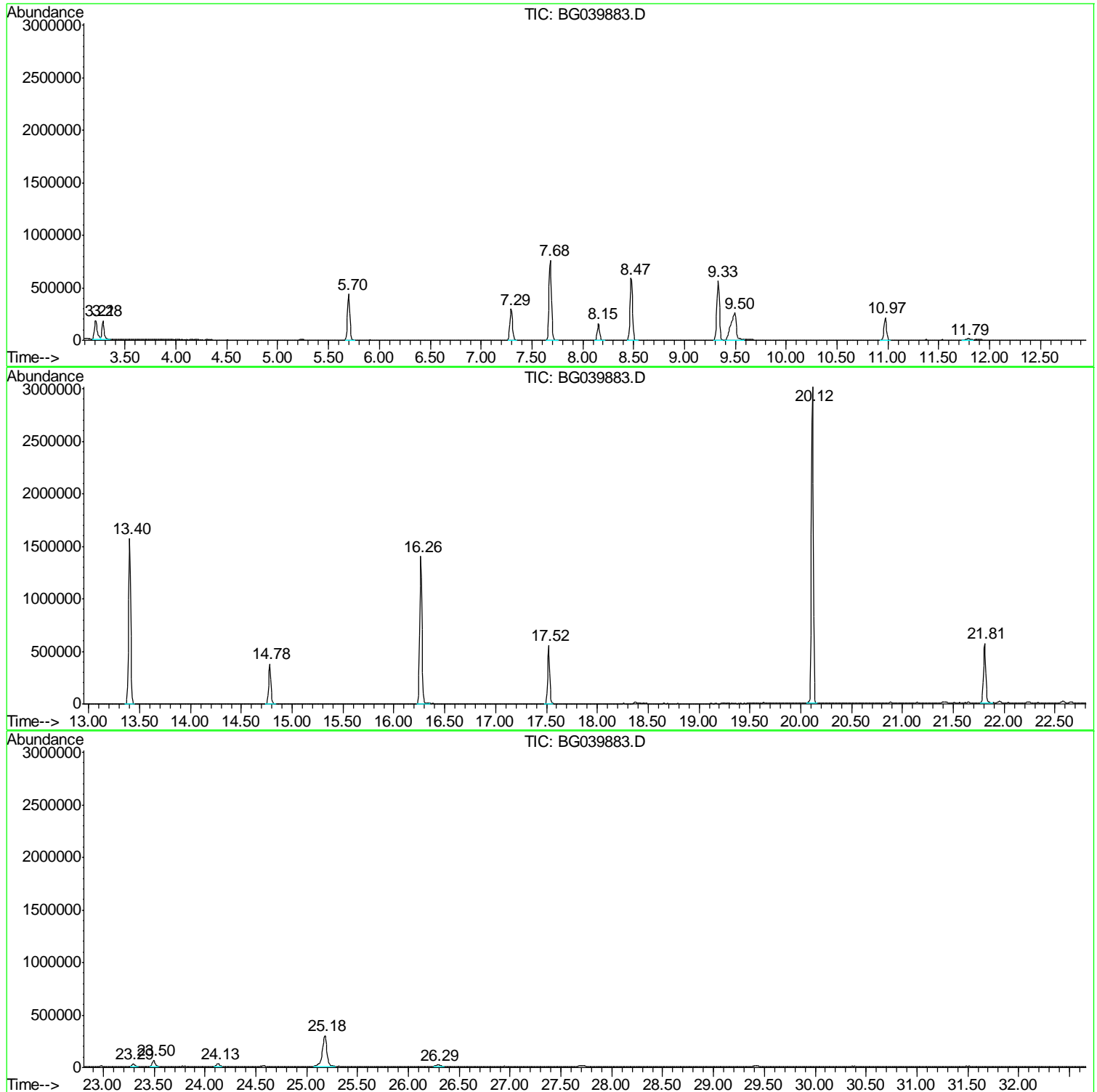
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Instrument :  
BNA\_G  
ClientSampleId :  
C-MW-10\_030719

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.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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Instrument :  
 BNA\_G  
 ClientSampled :  
 C-MW-10\_030719

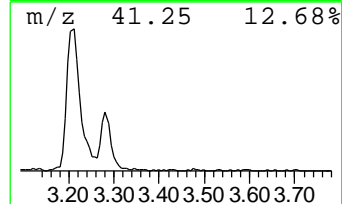
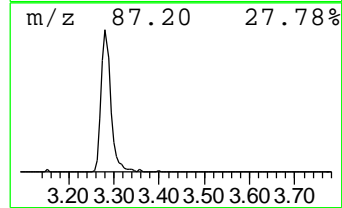
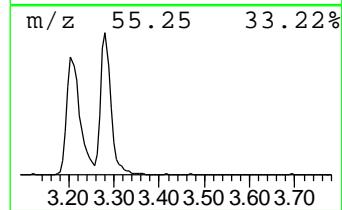
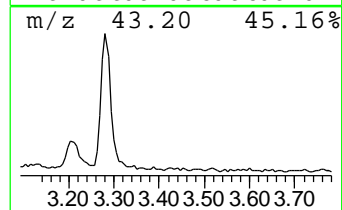
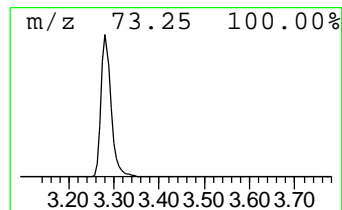
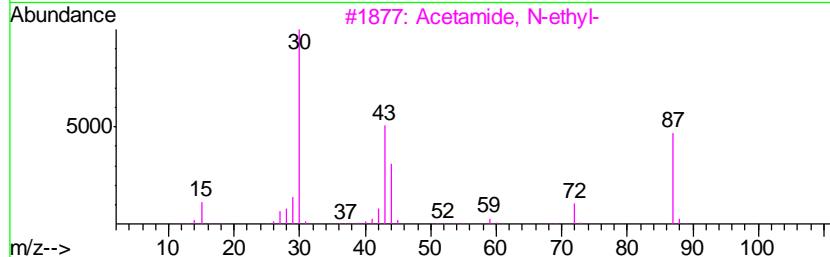
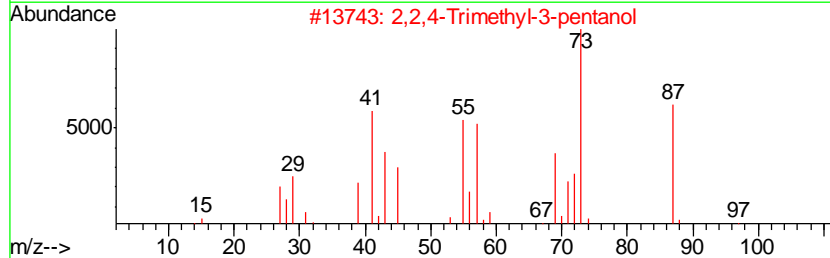
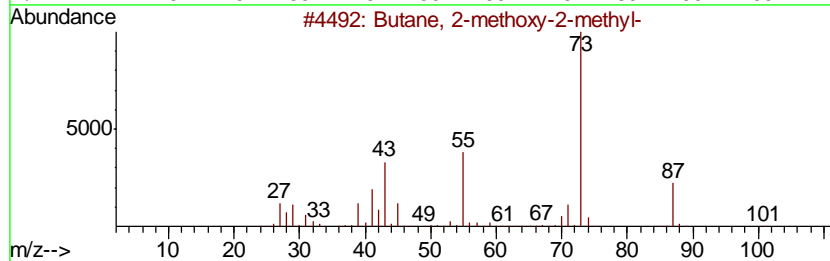
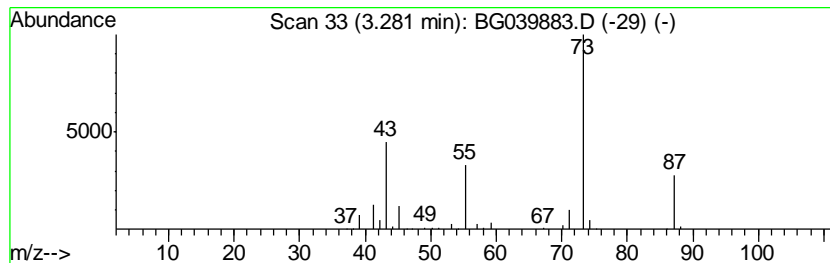
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.28	19.08 ng	260742	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	9



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M  
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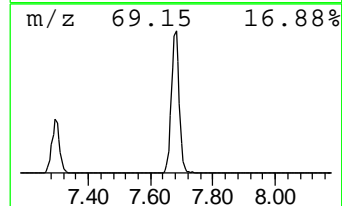
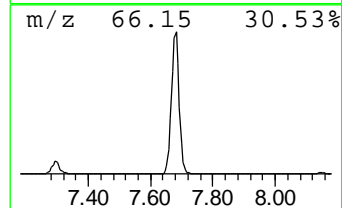
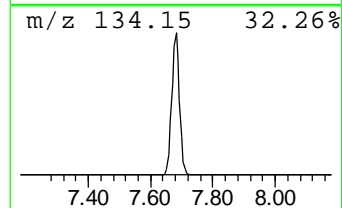
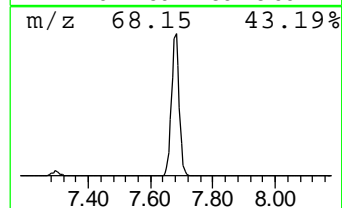
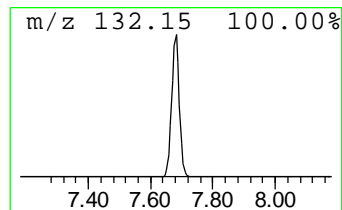
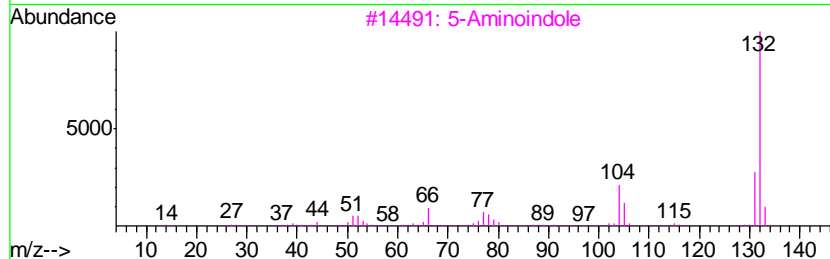
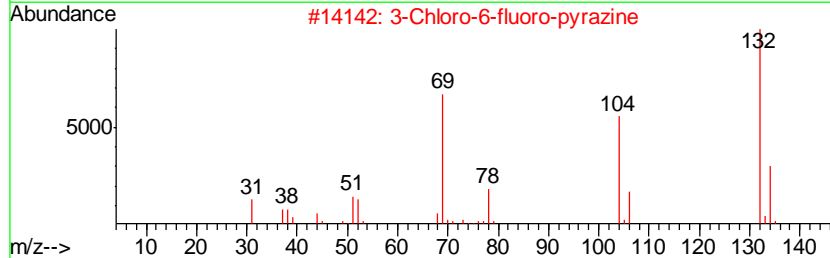
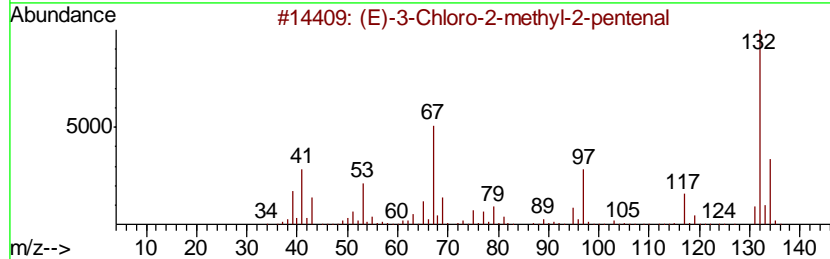
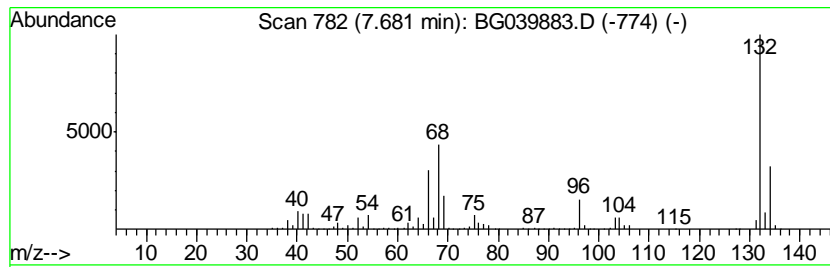
TIC Library : C:\Database\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	95.17 ng	1300910	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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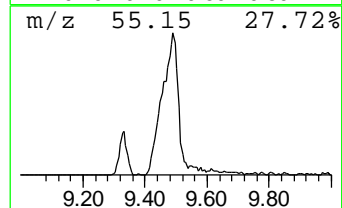
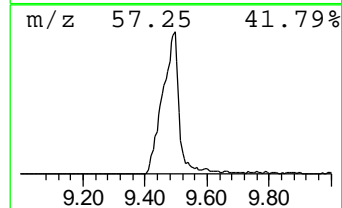
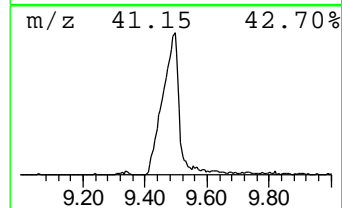
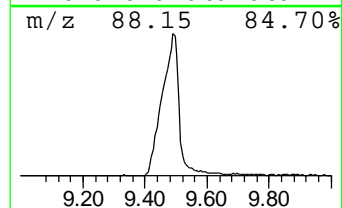
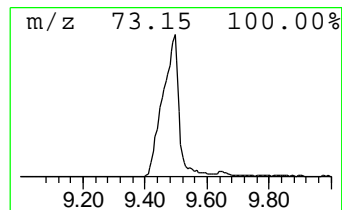
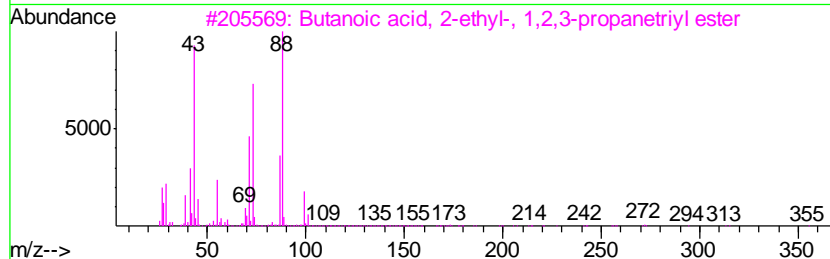
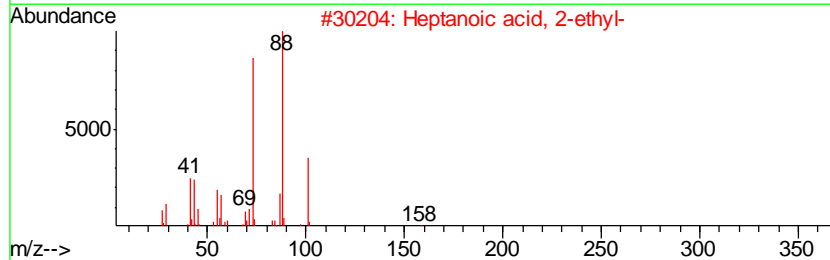
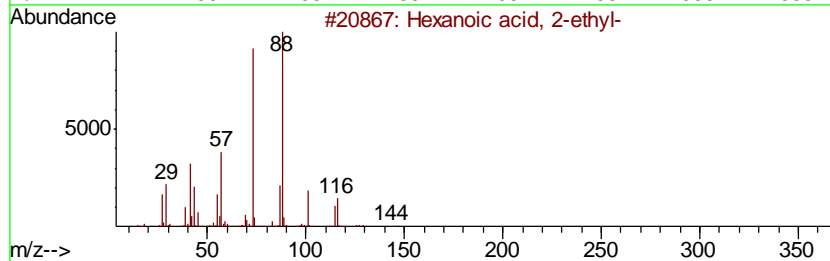
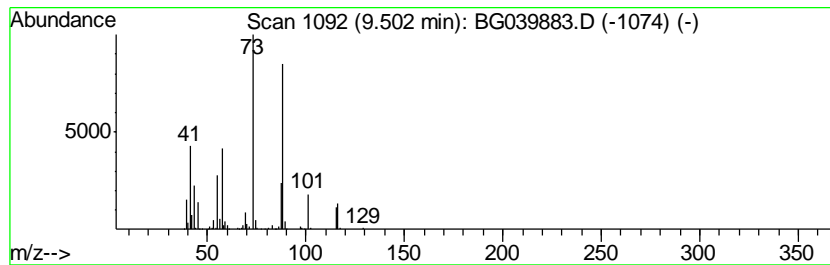
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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 Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.50	70.12 ng	958465	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2		Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	53
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	53
4		1,4-Dioxane	88	C4H8O2	000123-91-1	47
5		Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	47



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M  
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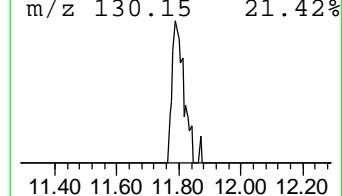
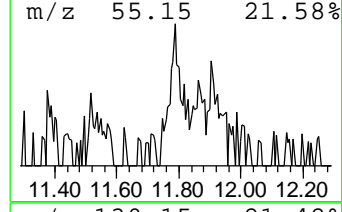
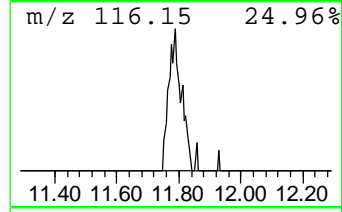
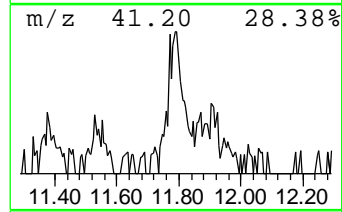
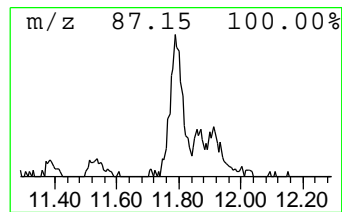
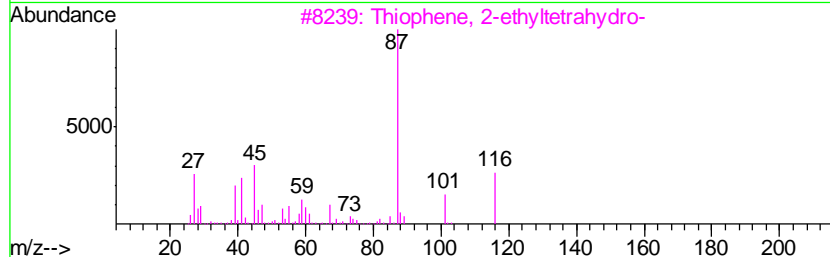
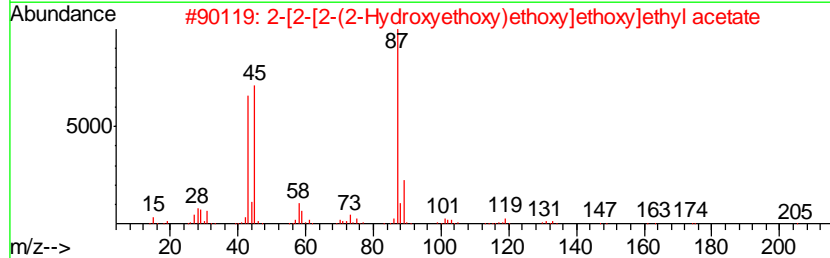
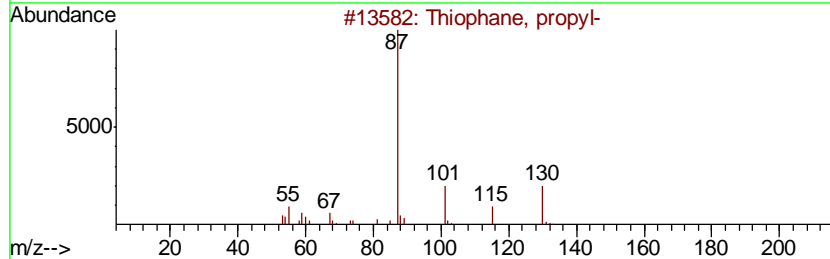
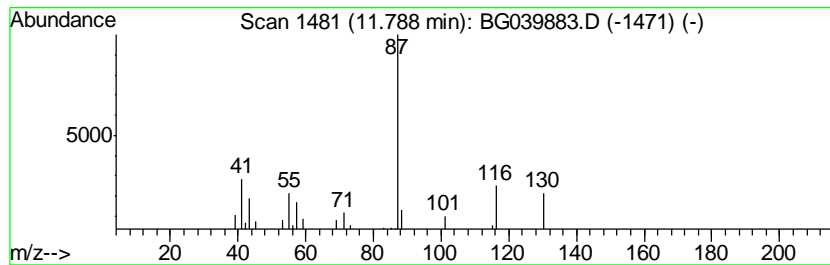
TIC Library : C:\Database\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 6 unknown11.79 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	2.19 ng	42854	Naphthalene-d8	10.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiophane, propyl-	130	C7H14S	001551-34-4	40
2		2-[2-[2-(2-Hydroxyethoxy)ethoxy]...]	236	C10H20O6	1000351-92-5	38
3		Thiophene, 2-ethyltetrahydro-	116	C6H12S	001551-32-2	38
4		Neodecanoic acid	172	C10H20O2	026896-20-8	36
5		3-Hexanol, 2,3-dimethyl-	130	C8H18O	004166-46-5	33



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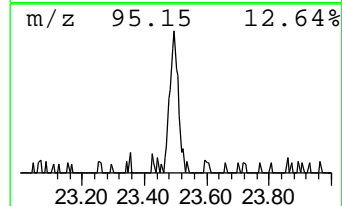
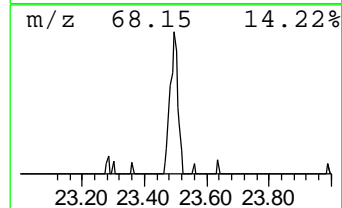
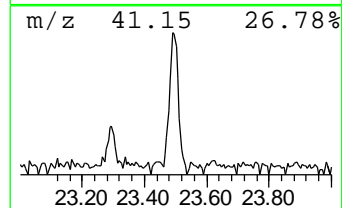
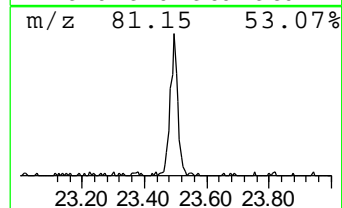
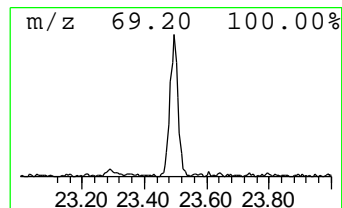
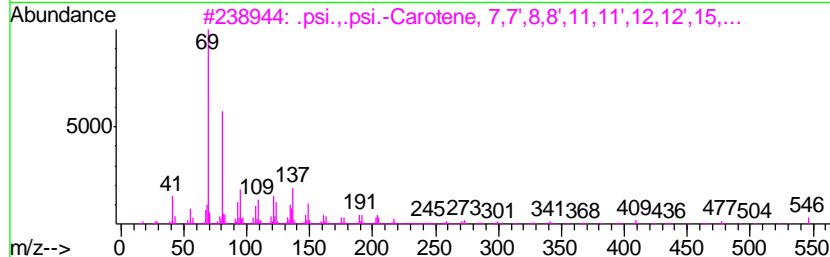
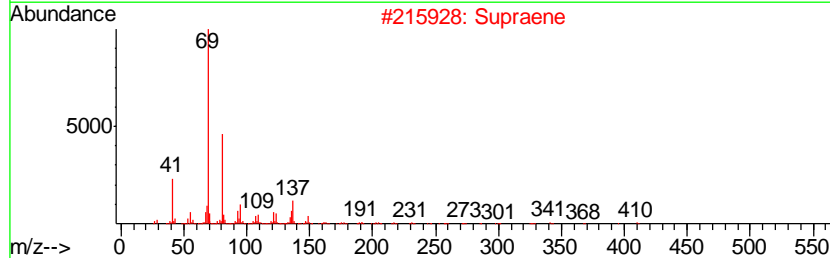
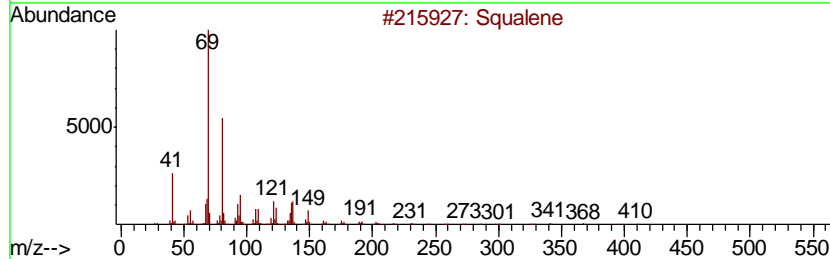
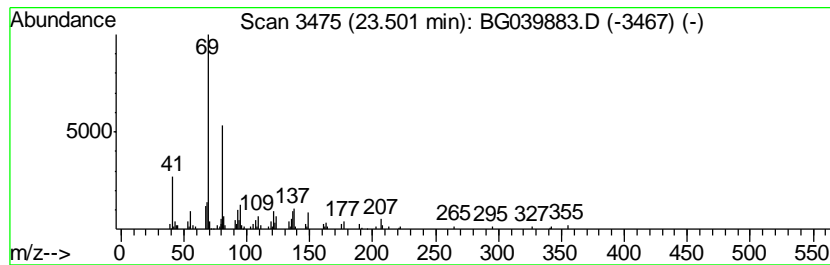
TIC Library : C:\Database\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.50	2.53 ng	118960	Perylene-d12	25.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	83
3		.psi...psi.-Carotene, 7,7',8,8',... 547	547	C40H66	000502-62-5	83
4		4,8,12-Tetradecatrienal, 5,9,13-... 248	248	C17H28O	066408-55-7	80
5		1,5,9-Decatriene, 2,3,5,8-tetram... 192	192	C14H24	230646-72-7	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.28	19.1 ng		260742	1	8.15	273377	20.0
unknown7.68	7.68	95.2 ng		1300910	1	8.15	273377	20.0
Hexanoic acid, 2-...	9.50	70.1 ng		958465	1	8.15	273377	20.0
unknown11.79	11.79	2.2 ng		42854	2	10.97	391774	20.0
Squalene	23.50	2.5 ng		118960	6	25.18	941870	20.0