

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_G\DATA\BG011518\
 Data File : BG032067.D
 Acq On : 16 Jan 2018 13:36
 Operator : SJ/JU
 Sample : J1123-02
 Misc :
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-4(30)

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_G\METHODS\8270-BG011218.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	3.410	14	21	32	rBV2	39748	111634	4.04%	0.702%
2	3.504	32	37	48	rVB2	25923	53619	1.94%	0.337%
3	5.684	404	408	422	rVB2	25550	46219	1.67%	0.291%
4	6.195	488	495	509	rBV	513530	882520	31.90%	5.550%
5	7.870	772	780	792	rBV	505573	953171	34.45%	5.994%
6	8.281	841	850	859	rBV	540227	992382	35.87%	6.241%
7	8.769	924	933	943	rVB	153656	276942	10.01%	1.742%
8	9.104	981	990	1001	rBV	429058	796916	28.81%	5.011%
9	9.962	1128	1136	1147	rBV	296290	563672	20.38%	3.545%
10	11.648	1415	1423	1435	rBV	189061	357958	12.94%	2.251%
11	12.905	1631	1637	1645	rBB	64713	104719	3.79%	0.659%
12	14.027	1818	1828	1840	rVB	1052814	1673250	60.48%	10.522%
13	14.821	1957	1963	1971	rVB	266111	395499	14.30%	2.487%
14	15.396	2053	2061	2071	rVB2	321418	540310	19.53%	3.398%
15	16.724	2280	2287	2296	rBV	587828	930846	33.65%	5.854%
16	16.871	2304	2312	2320	rBV	924609	1458682	52.73%	9.173%
17	17.382	2392	2399	2405	rBV	20218	35515	1.28%	0.223%
18	18.128	2520	2526	2534	rBV2	460210	725882	26.24%	4.565%
19	18.945	2659	2665	2681	rBV2	90989	157820	5.70%	0.992%
20	20.179	2871	2875	2879	rBV3	30128	45168	1.63%	0.284%
21	20.661	2951	2957	2964	rBV	2021450	2766453	100.00%	17.397%
22	22.006	3180	3186	3192	rBV3	53745	96047	3.47%	0.604%
23	22.465	3256	3264	3274	rBV2	507478	973230	35.18%	6.120%
24	26.178	3884	3896	3912	rBV2	290484	963803	34.84%	6.061%

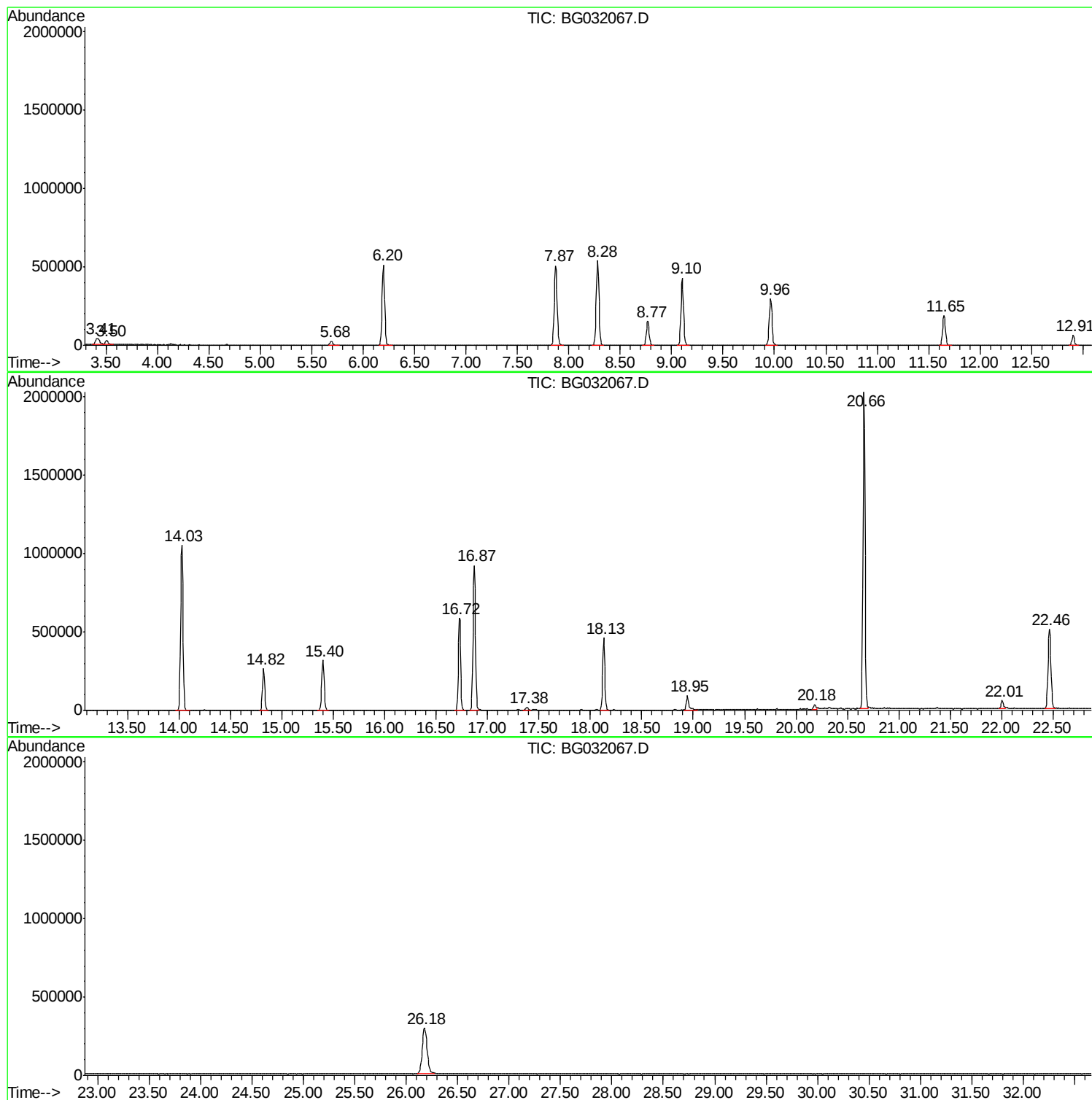
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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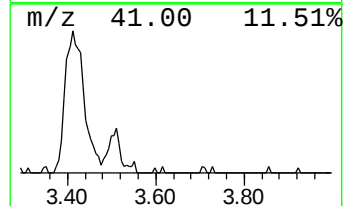
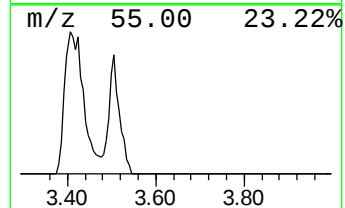
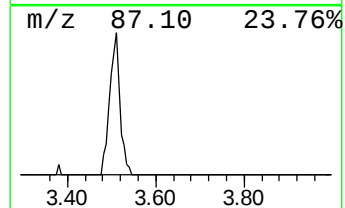
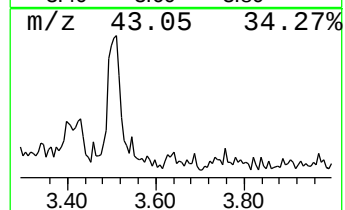
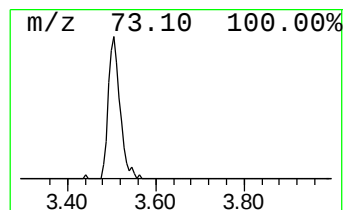
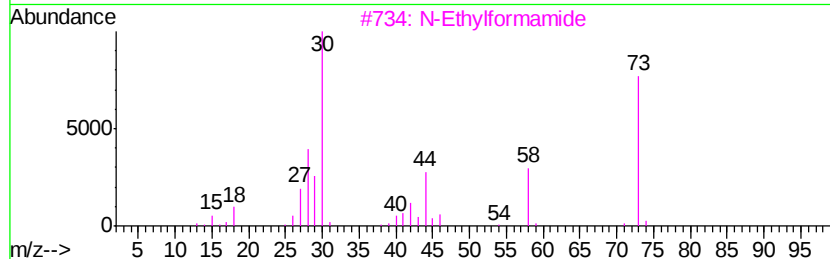
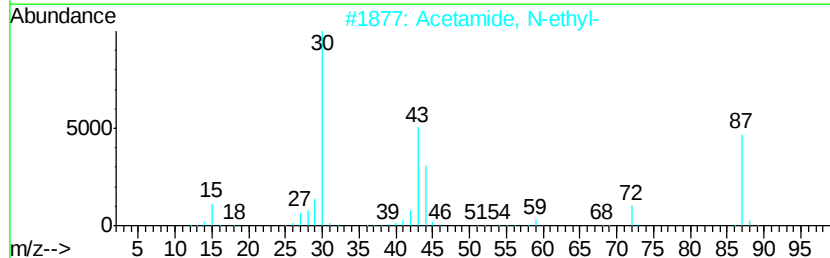
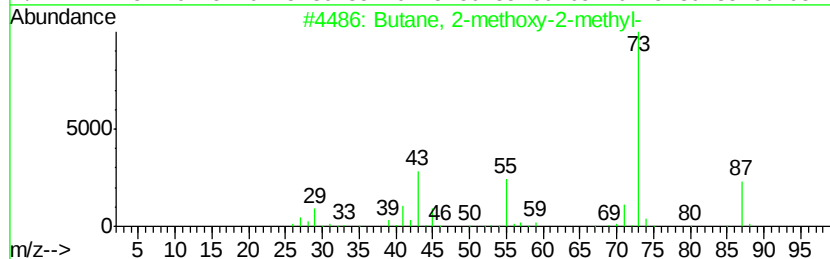
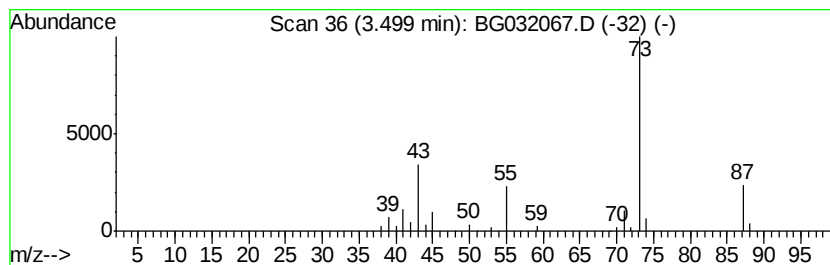
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	3.87 ng	53619	1,4-Dichlorobenzene-d4	8.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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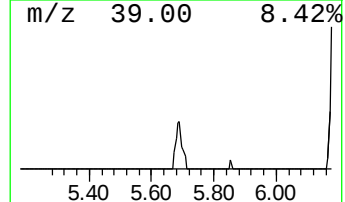
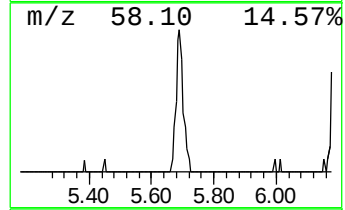
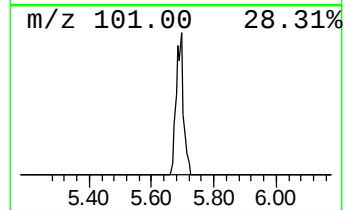
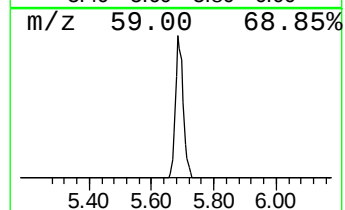
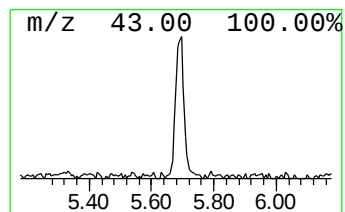
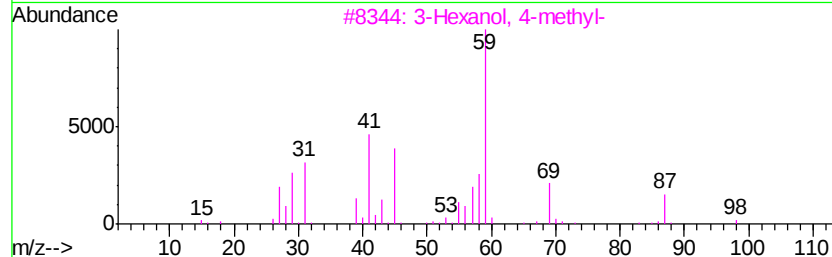
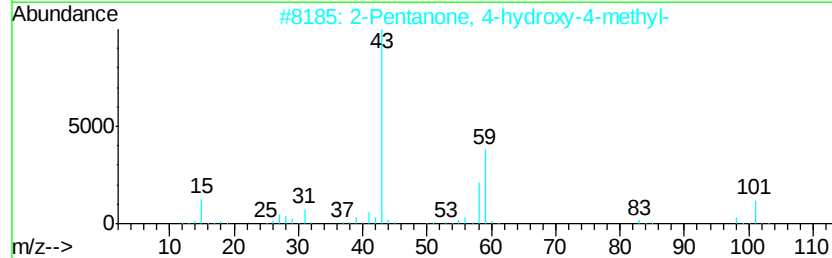
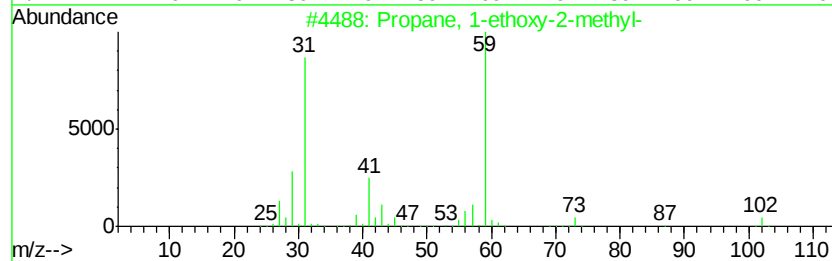
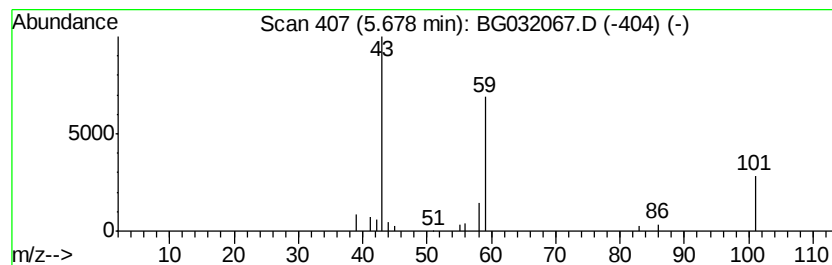
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Peak Number 3 unknown5.68 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	3.34 ng	46219	1,4-Dichlorobenzene-d4	8.77

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	43
2			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			3-Hexanol	102	C6H14O	000623-37-0	33
5			Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	28



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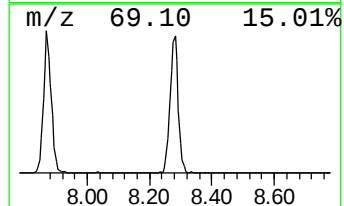
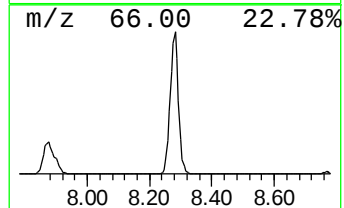
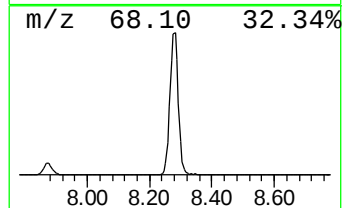
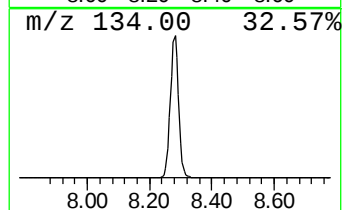
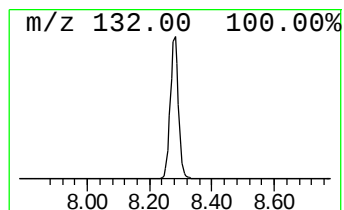
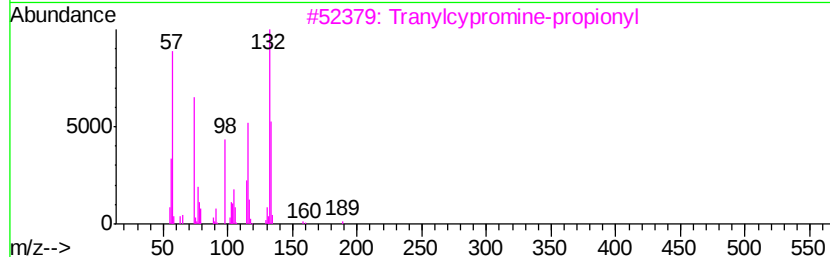
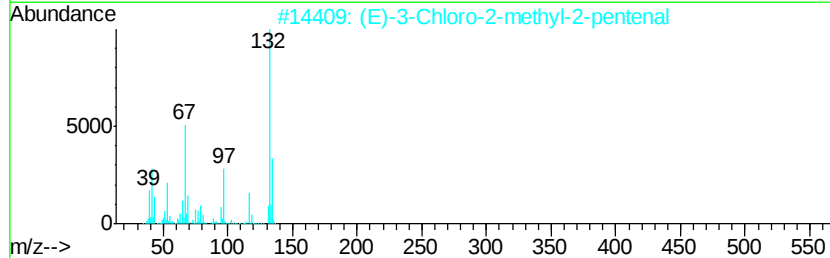
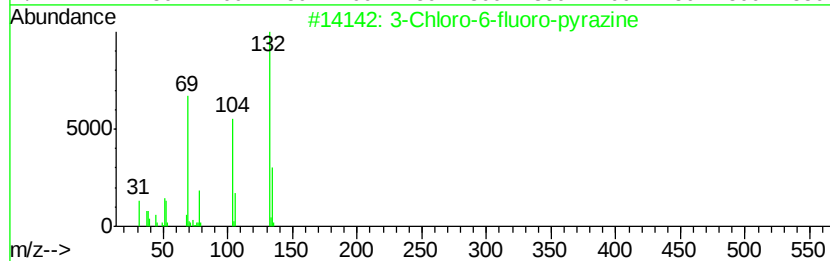
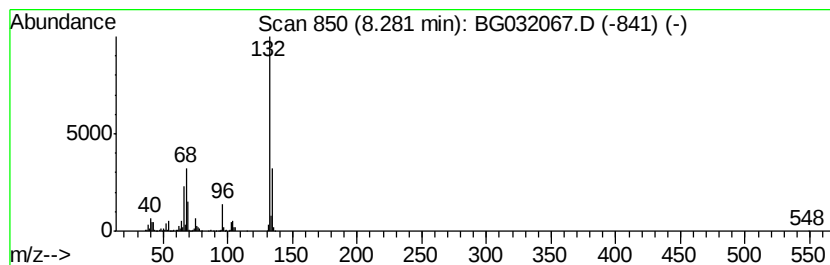
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Peak Number 4 unknown8.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	71.67 ng	992382	1,4-Dichlorobenzene-d4	8.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		5-Aminoindole	132	C8H8N2	005192-03-0	16
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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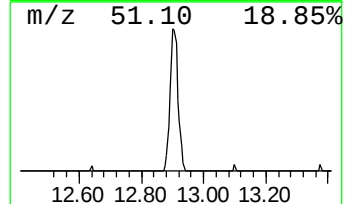
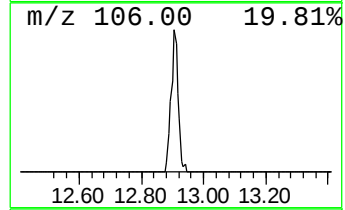
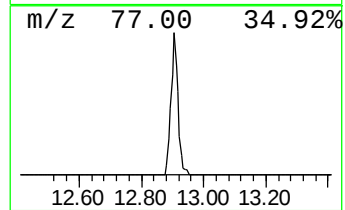
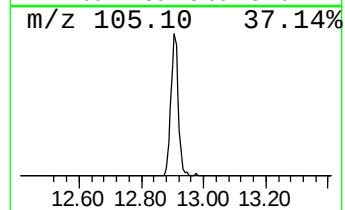
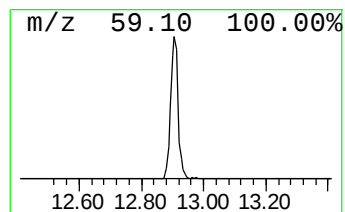
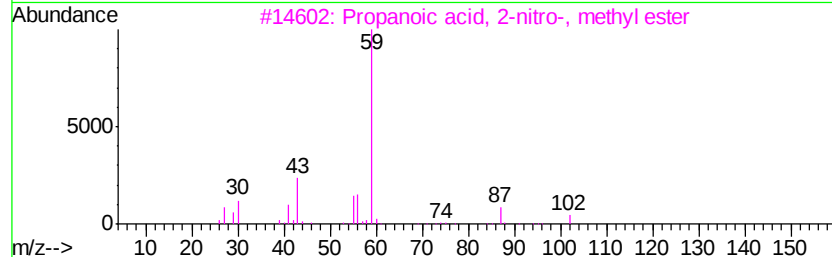
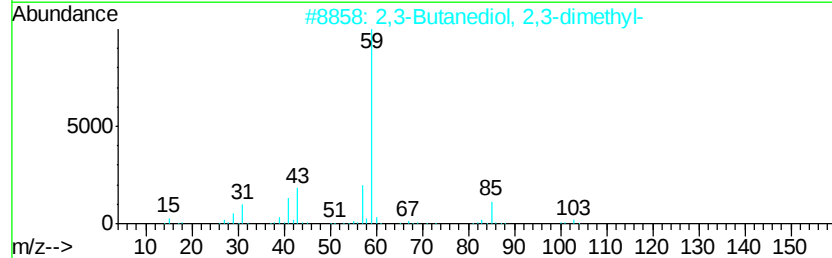
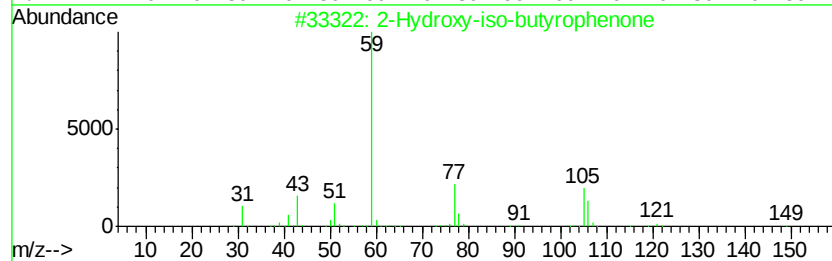
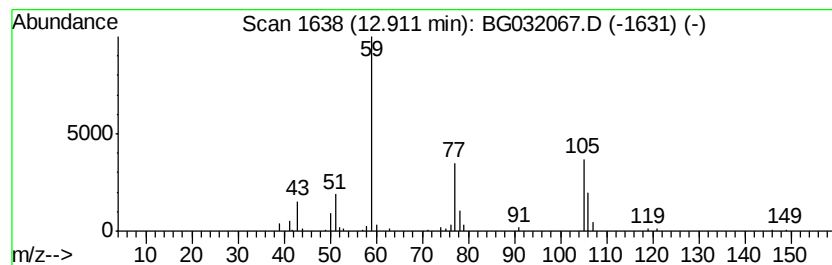
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Peak Number 6 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	5.85 ng	104719	Napthalene-d8	11.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	72
2		2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	9
3		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9
4		Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
5		Acetamide	59	C2H5NO	000060-35-5	5



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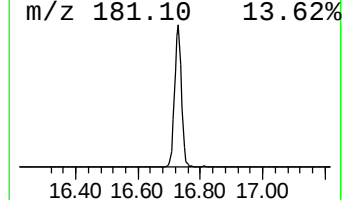
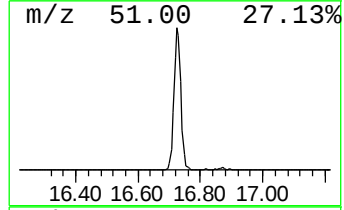
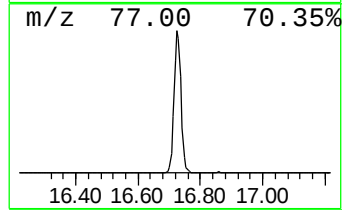
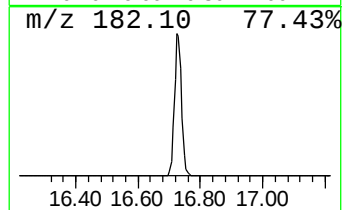
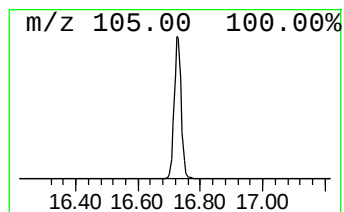
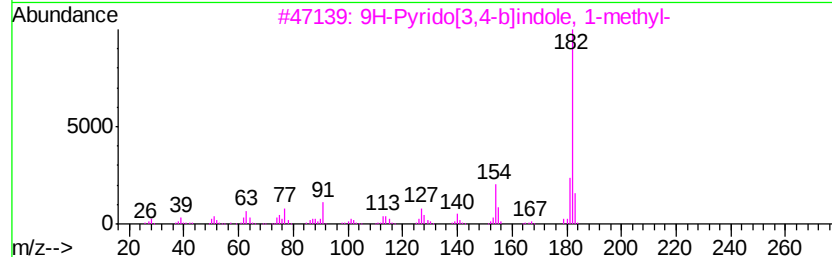
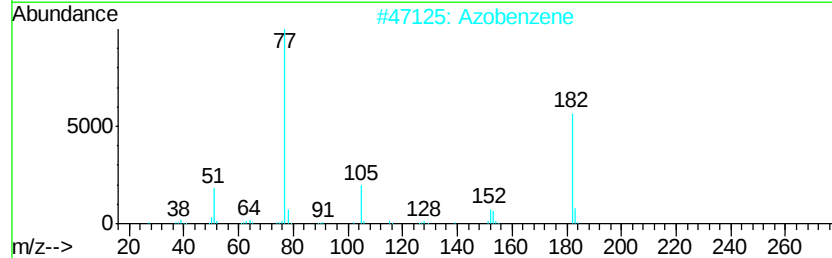
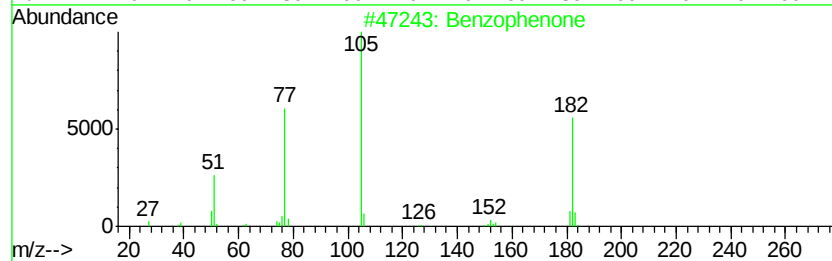
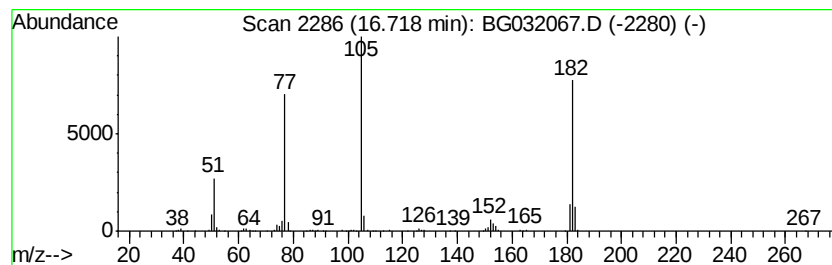
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Peak Number 7 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.72	34.46 ng	930846	Acenaphthene-d10	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		Azobenzene	182	C12H10N2	000103-33-3	72
3		9H-Pyrido[3,4-b]indole, 1-methyl-	182	C12H10N2	000486-84-0	43
4		1-Methyl-1,6-diazaplenalene	182	C12H10N2	079691-99-9	38
5		Vinyl benzoate	148	C9H8O2	000769-78-8	35



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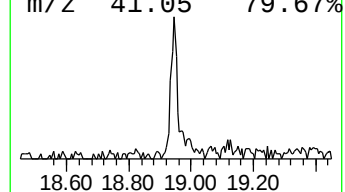
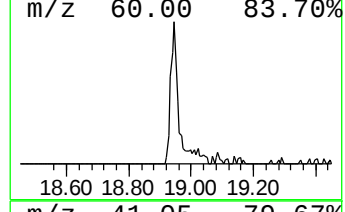
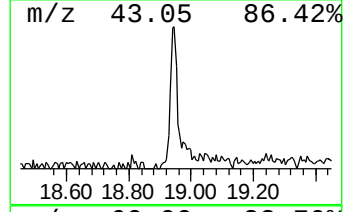
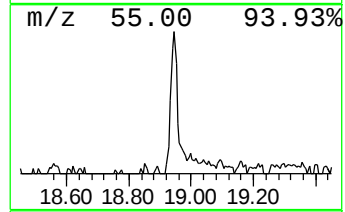
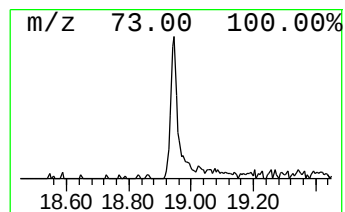
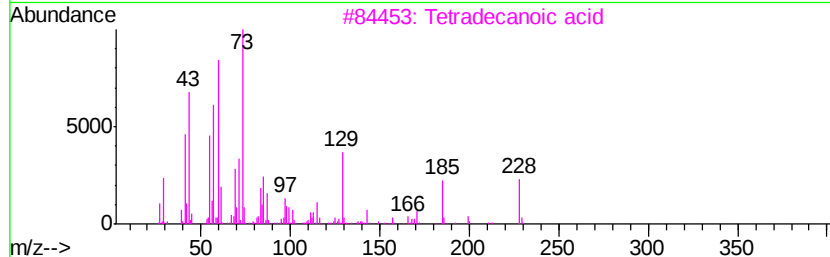
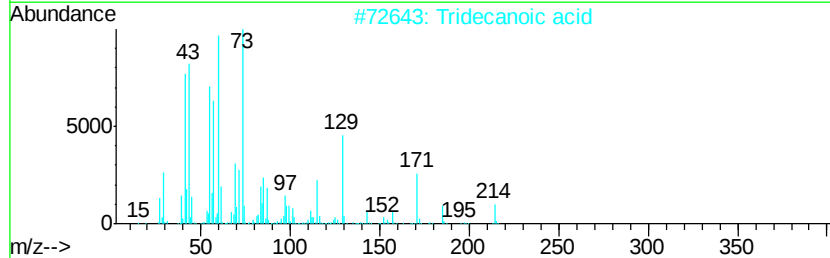
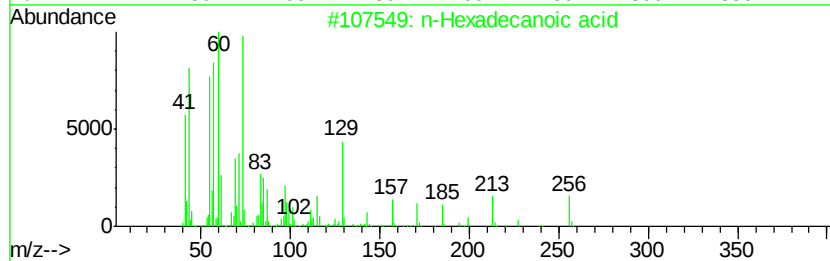
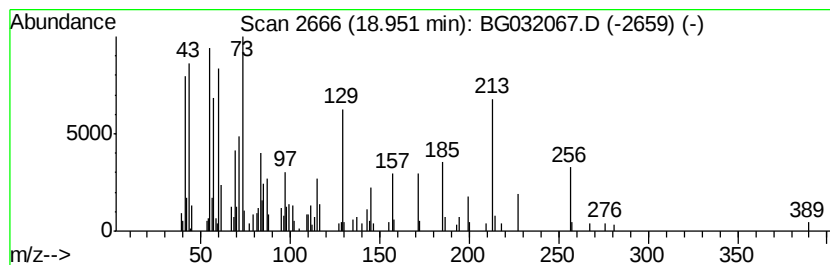
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.95	4.35 ng	157820	Phenanthrene-d10	18.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	92
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4		n-Decanoic acid	172	C10H20O2	000334-48-5	50
5		Dodecanoic acid	200	C12H24O2	000143-07-7	38



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_G\DATA\BG011518\
Data File : BG032067.D
Acq On : 16 Jan 2018 13:36
Operator : SJ/JU
Sample : J1123-02
Misc :
ALS Vial : 33 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-4(30)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.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
Butane, 2-methoxy...	3.50	3.9	ng	53619	1	8.77	276942	20.0
unknown5.68	5.68	3.3	ng	46219	1	8.77	276942	20.0
unknown8.28	8.28	71.7	ng	992382	1	8.77	276942	20.0
2-Hydroxy-iso-but...	12.91	5.8	ng	104719	2	11.65	357958	20.0
Benzophenone	16.72	34.5	ng	930846	3	15.40	540310	20.0
n-Hexadecanoic acid	18.95	4.3	ng	157820	4	18.13	725882	20.0