

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111519\
 Data File : BG043658.D
 Acq On : 15 Nov 2019 19:54
 Operator : JU
 Sample : PB124785BL
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB124785BL

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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	3.152	6	11	27	rVB	300766	466580	17.61%	5.161%
2	3.881	131	135	144	rBV	17748	27576	1.04%	0.305%
3	4.492	233	239	247	rBV	38632	58657	2.21%	0.649%
4	5.097	336	342	348	rBV	21412	32134	1.21%	0.355%
5	5.584	416	425	439	rBV	153665	287084	10.84%	3.176%
6	7.188	692	698	710	rBV2	90832	190717	7.20%	2.110%
7	7.535	750	757	771	rBV	246951	472941	17.85%	5.232%
8	7.993	828	835	845	rBV	82290	149214	5.63%	1.651%
9	8.317	882	890	907	rBV	314463	565827	21.36%	6.259%
10	9.157	1026	1033	1049	rBV2	190531	413072	15.59%	4.570%
11	10.802	1306	1313	1323	rBV	77708	175632	6.63%	1.943%
12	13.246	1722	1729	1741	rBV	686069	1165140	43.97%	12.889%
13	14.627	1958	1964	1977	rBV2	155585	292540	11.04%	3.236%
14	16.119	2211	2218	2237	rBV	361314	739773	27.92%	8.184%
15	17.371	2425	2431	2445	rBV	238530	444229	16.77%	4.914%
16	19.979	2869	2875	2890	rBV	1845882	2649595	100.00%	29.311%
17	21.636	3149	3157	3170	rBV	302090	598253	22.58%	6.618%
18	23.881	3533	3539	3545	rBV7	13626	27271	1.03%	0.302%
19	24.827	3690	3700	3712	rBV3	81181	283500	10.70%	3.136%

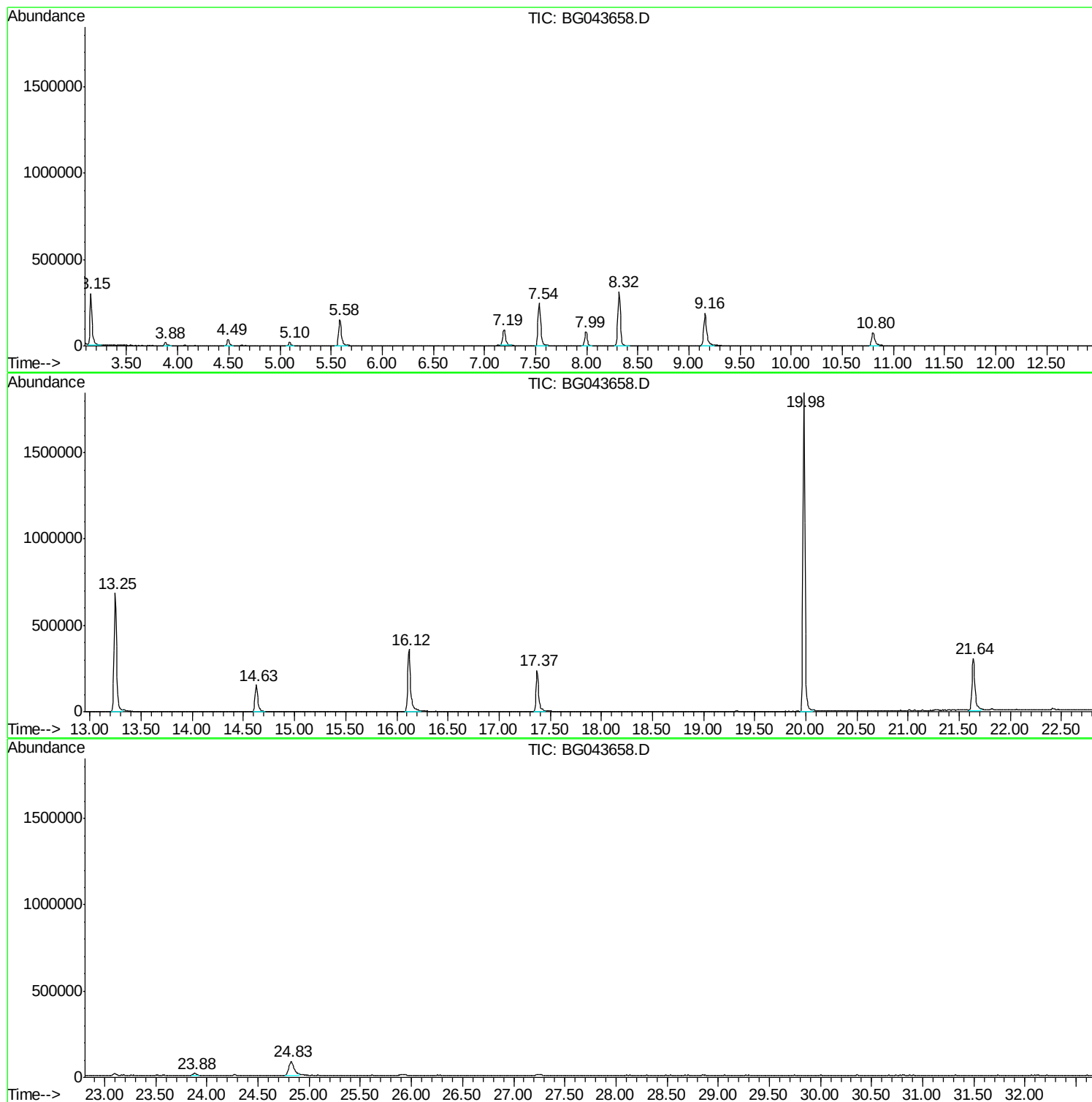
Sum of corrected areas: 9039735

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.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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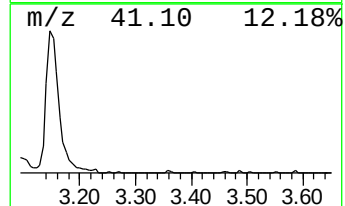
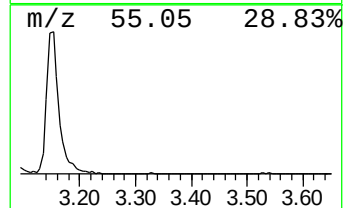
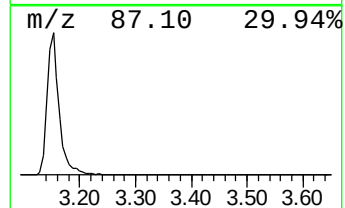
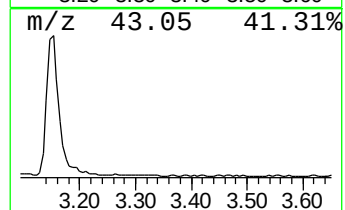
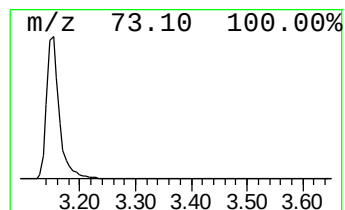
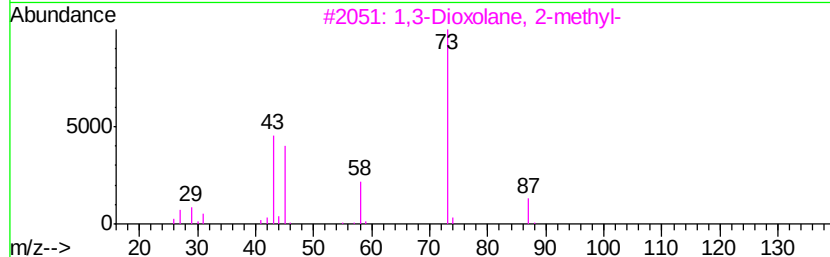
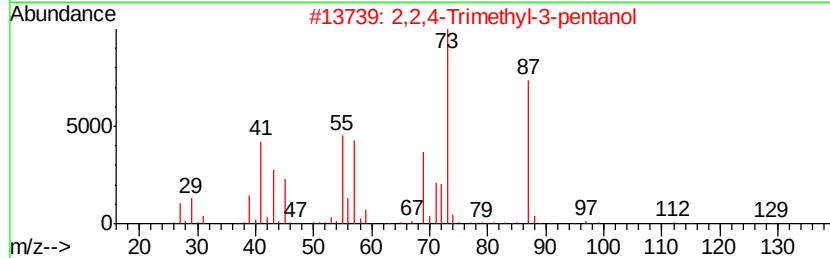
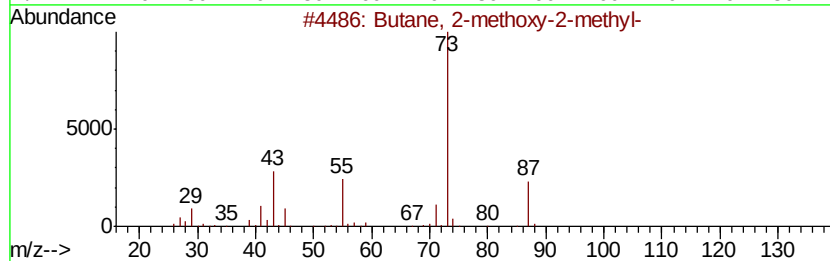
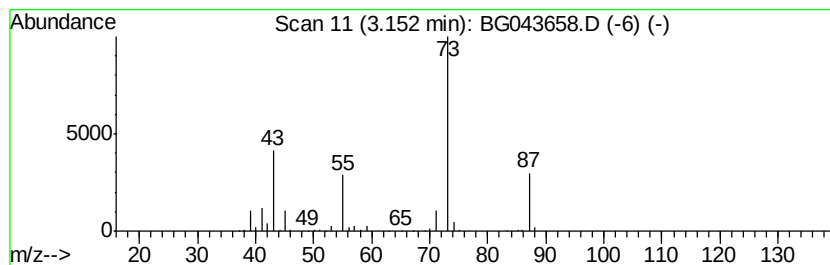
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	62.54 ng	466580	1,4-Dichlorobenzene-d4	7.99

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	33
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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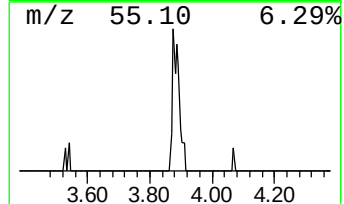
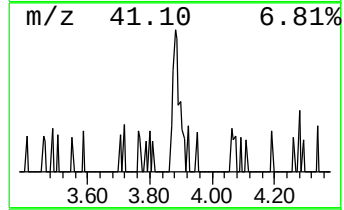
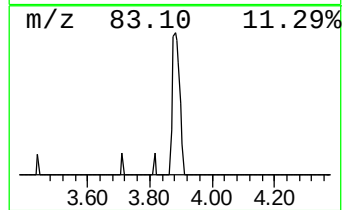
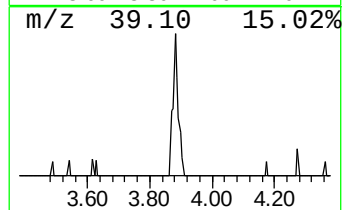
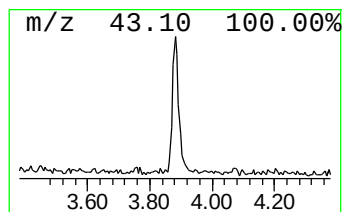
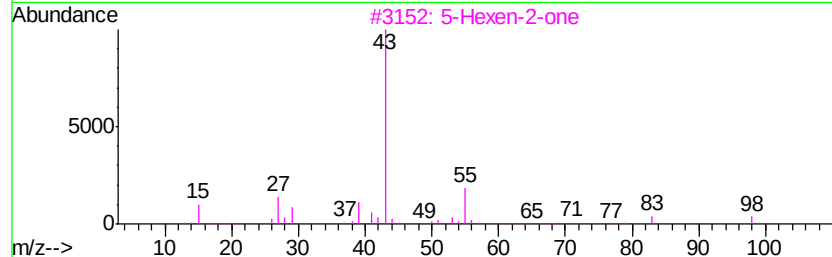
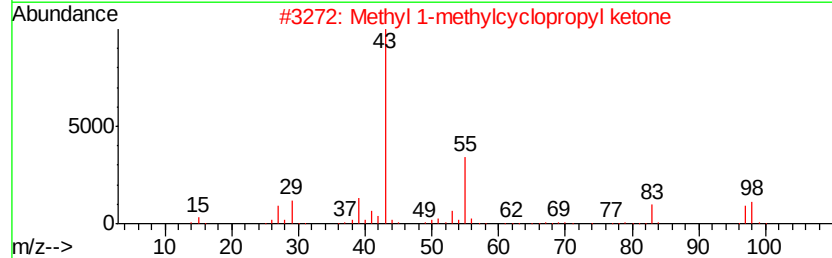
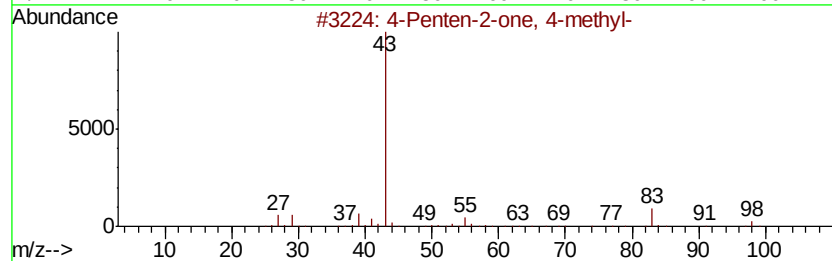
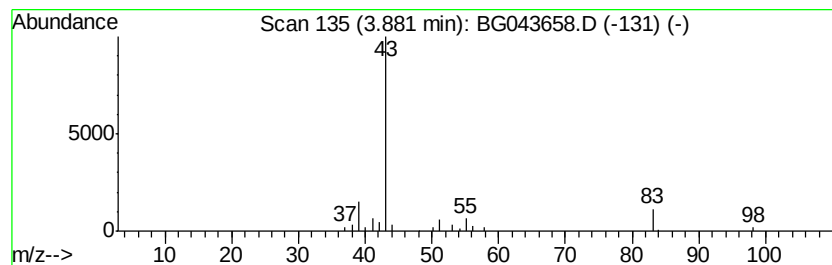
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.88	3.70 ng	27576	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	64
2		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	49
3		5-Hexen-2-one	98	C6H10O	000109-49-9	28
4		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
5		2-Vinylethyl acetate	114	C6H10O2	001576-84-7	9



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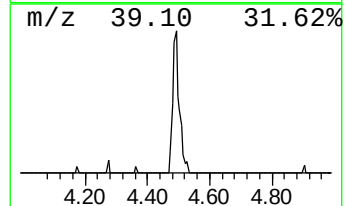
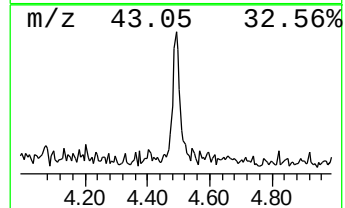
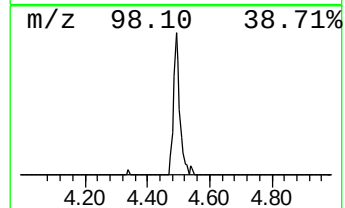
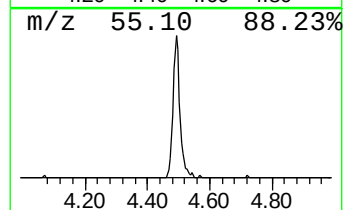
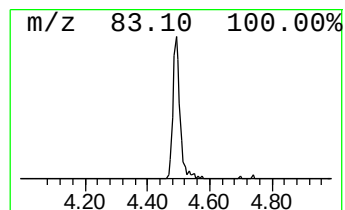
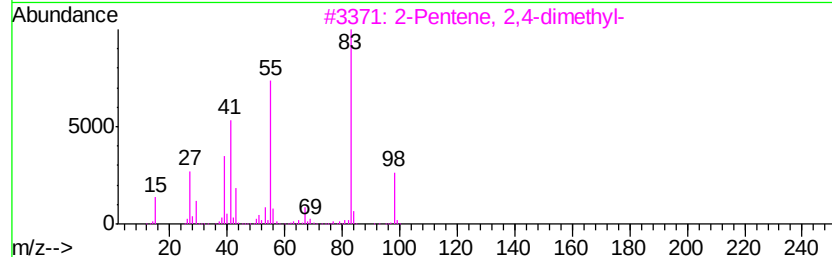
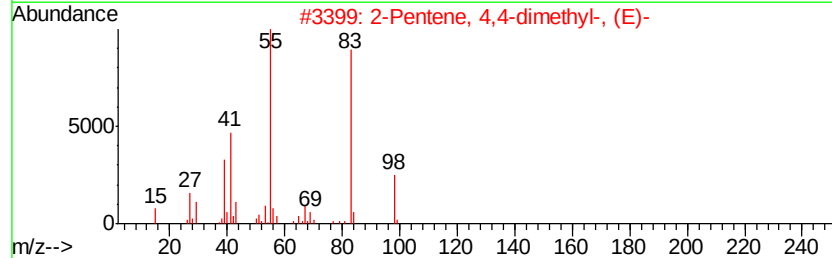
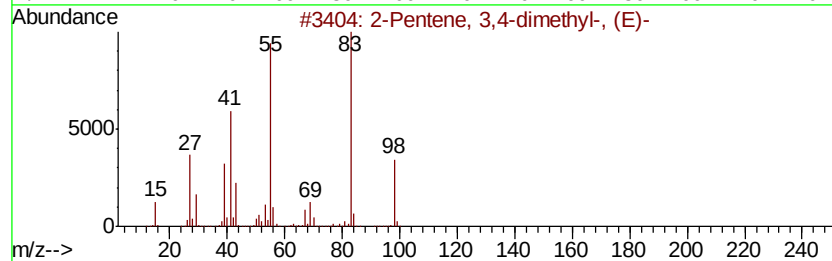
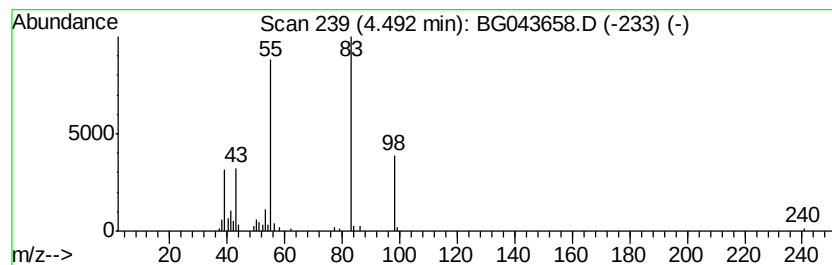
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentene, 3,4-dimethyl-, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	7.86 ng	58657	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
2		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4		3-Hexen-2-one	98	C6H10O	000763-93-9	86
5		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	80



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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
PB124785BL

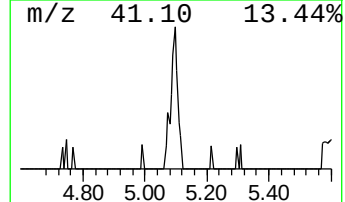
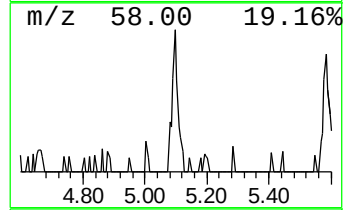
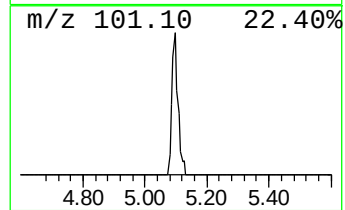
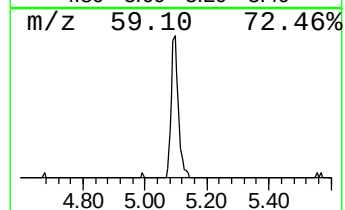
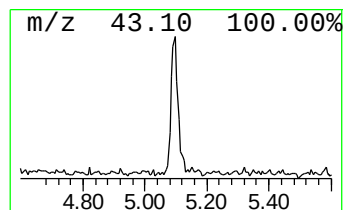
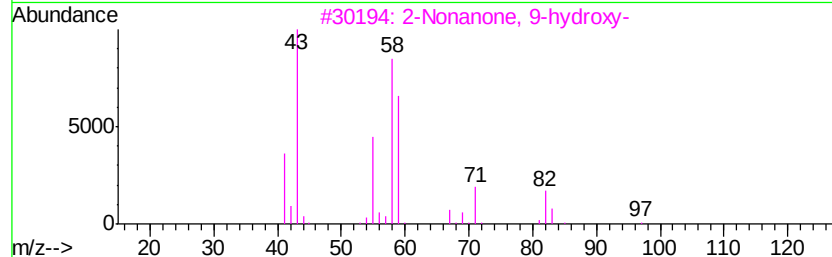
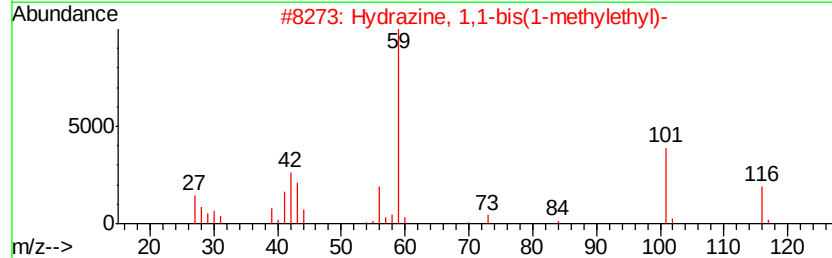
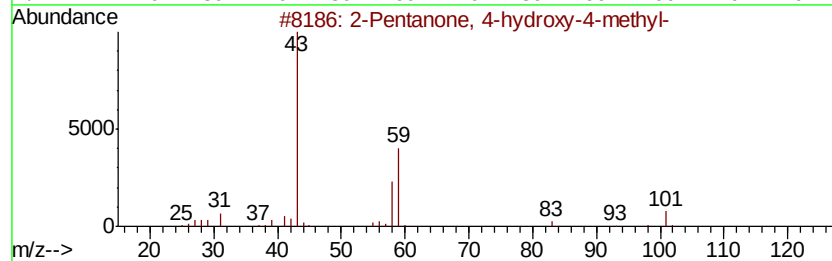
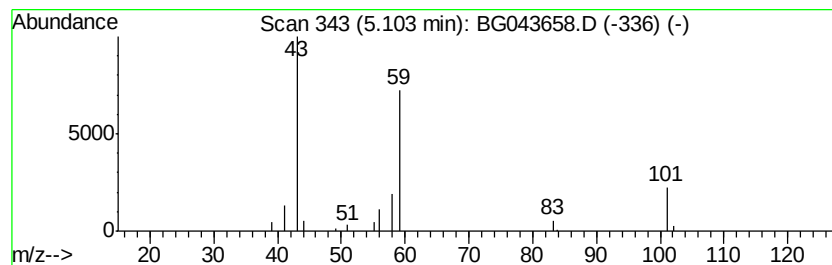
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	4.31 ng	32134	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	37
3		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	25
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Acetone	58	C3H6O	000067-64-1	9



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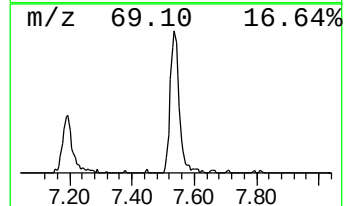
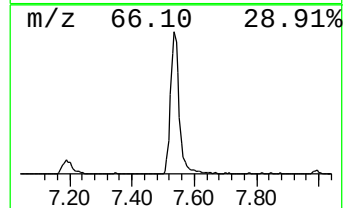
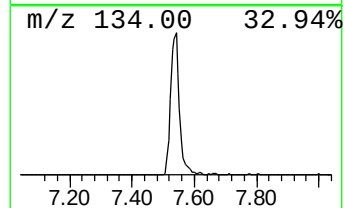
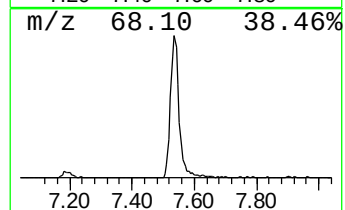
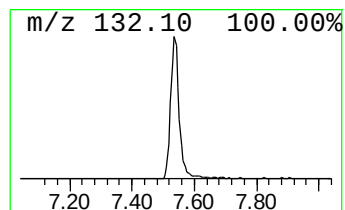
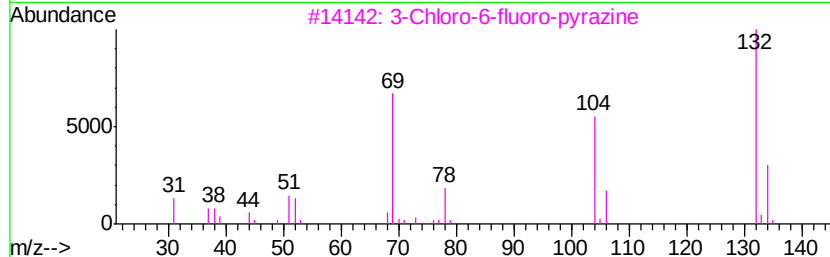
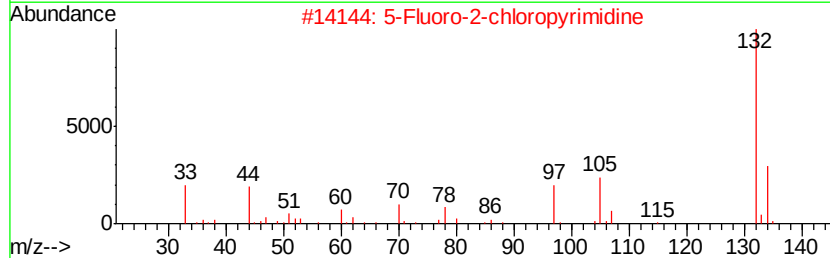
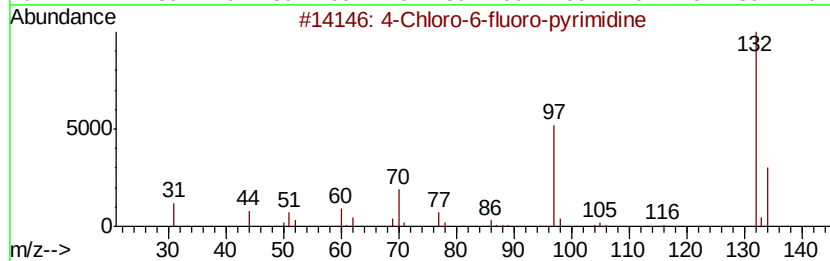
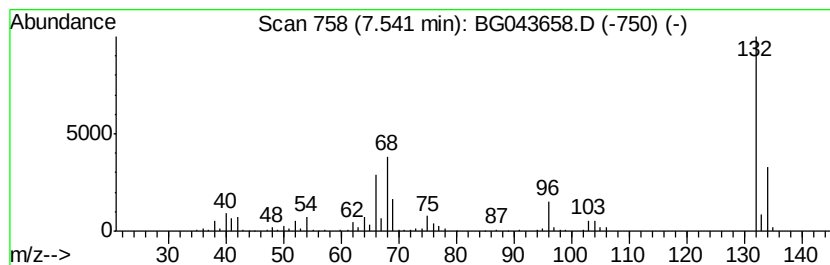
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown7.54 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	63.39 ng	472941	1,4-Dichlorobenzene-d4	7.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
4		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.15	62.5	ng	466580	1	7.99	149214	20.0
4-Penten-2-one, 4...	3.88	3.7	ng	27576	1	7.99	149214	20.0
2-Pentene, 3,4-di...	4.49	7.9	ng	58657	1	7.99	149214	20.0
2-Pentanone, 4-hy...	5.10	4.3	ng	32134	1	7.99	149214	20.0
unknown7.54	7.54	63.4	ng	472941	1	7.99	149214	20.0