

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120215\
 Data File : BG019846.D
 Acq On : 2 Dec 2015 22:35
 Operator : UM/NP
 Sample : G4585-11
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DUP3-112415

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_G\METHODS\8270-BG120215.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	2.879	5	7	9	rVB	2537331	1770587	69.22%	14.120%
2	3.143	47	52	63	rBV3	44181	94406	3.69%	0.753%
3	3.237	63	68	75	rVV	167535	246507	9.64%	1.966%
4	4.595	291	299	307	rBV	60786	88839	3.47%	0.708%
5	5.206	397	403	411	rVB	79915	118770	4.64%	0.947%
6	5.670	475	482	492	rVB	415149	645477	25.24%	5.147%
7	7.274	746	755	764	rBV	396142	662859	25.92%	5.286%
8	7.656	812	820	828	rBV	453642	755717	29.55%	6.027%
9	8.132	894	901	907	rBV	84418	137646	5.38%	1.098%
10	8.455	949	956	964	rVB	339553	569545	22.27%	4.542%
11	9.295	1091	1099	1108	rVB	291871	505921	19.78%	4.035%
12	10.946	1373	1380	1388	rBV	108640	193018	7.55%	1.539%
13	13.390	1789	1796	1802	rBV	812501	1264611	49.44%	10.085%
14	14.759	2022	2029	2037	rVB2	184107	292968	11.45%	2.336%
15	16.240	2275	2281	2287	rBV	800368	1179775	46.12%	9.408%
16	17.503	2489	2496	2502	rBV	295709	440153	17.21%	3.510%
17	20.112	2934	2940	2945	rVB	1983228	2557797	100.00%	20.397%
18	21.786	3219	3225	3232	rBV	373964	593404	23.20%	4.732%
19	25.094	3779	3788	3799	rVB2	139548	421788	16.49%	3.364%

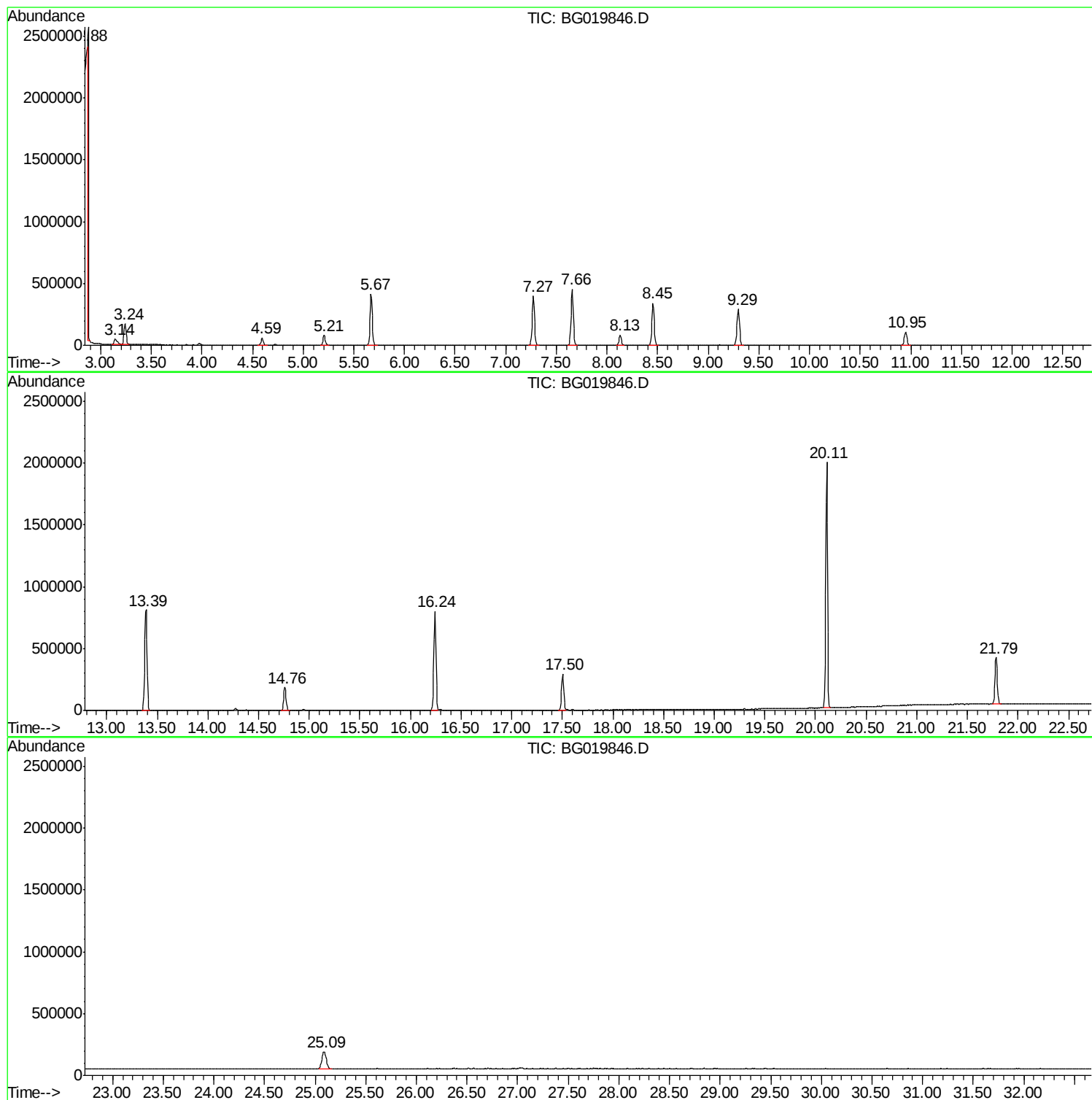
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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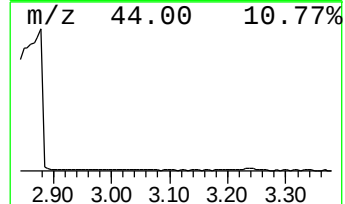
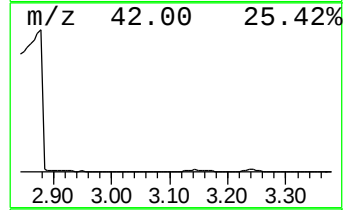
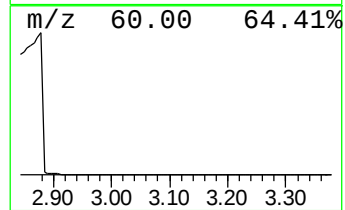
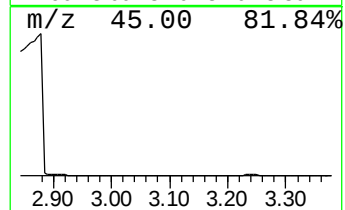
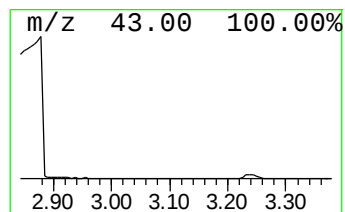
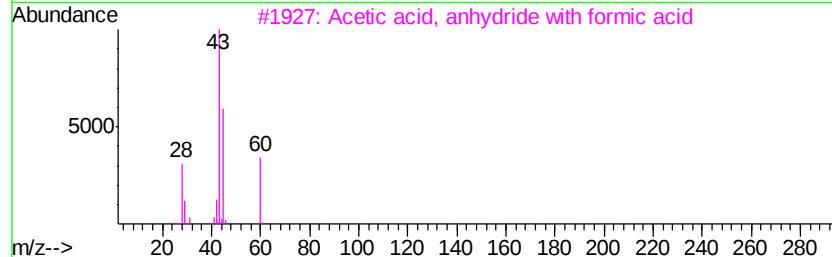
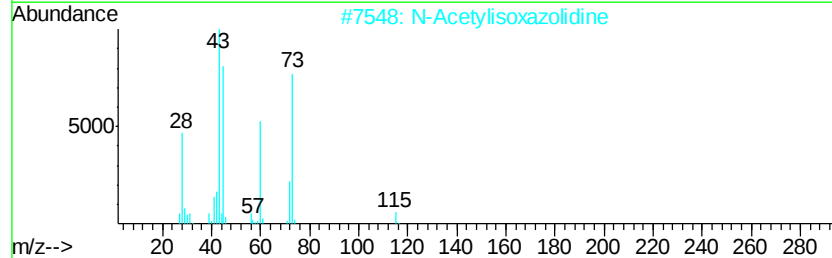
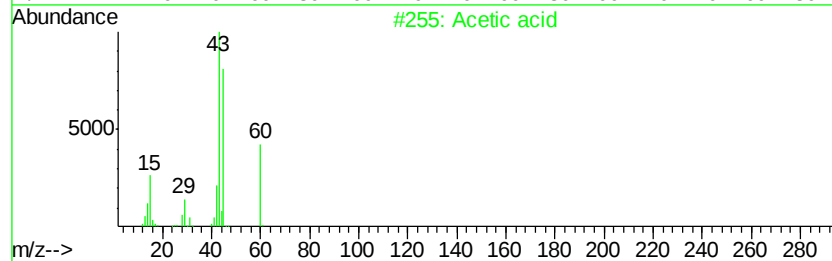
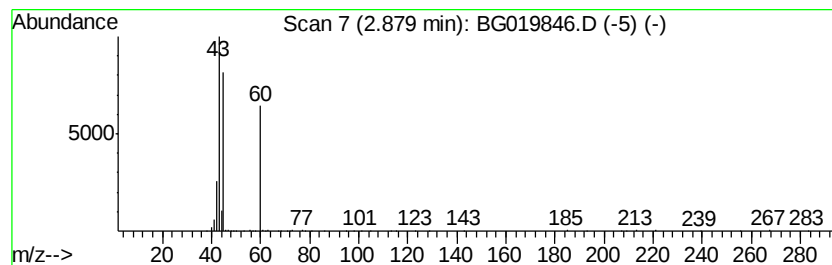
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	257.27 ng	1770590	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid	60	C2H4O2	000064-19-7	83
2		N-Acetylisoaxazolidine	115	C5H9N02	115615-36-6	43
3		Acetic acid, anhydride with form...	88	C3H4O3	002258-42-6	9
4		Cyclohexan-1,4,5-triol-3-one-1-c...	190	C7H10O6	1000128-45-5	9
5		Ammonium acetate	77	C2H7N02	000631-61-8	9



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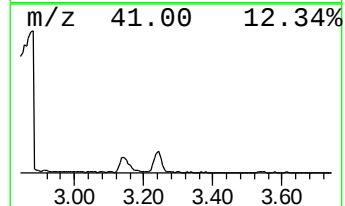
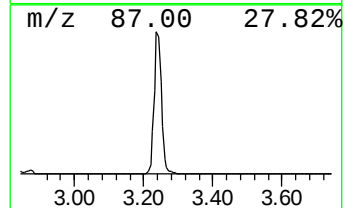
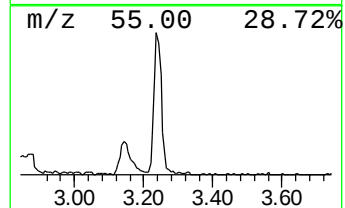
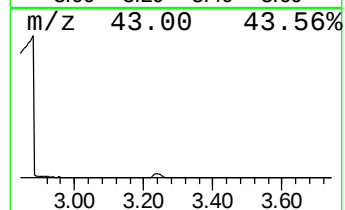
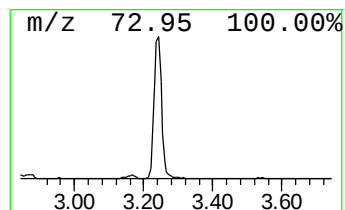
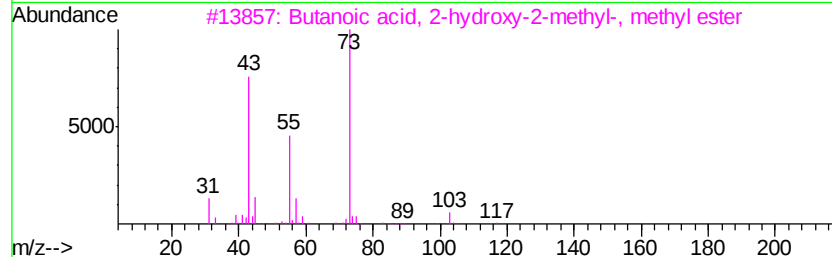
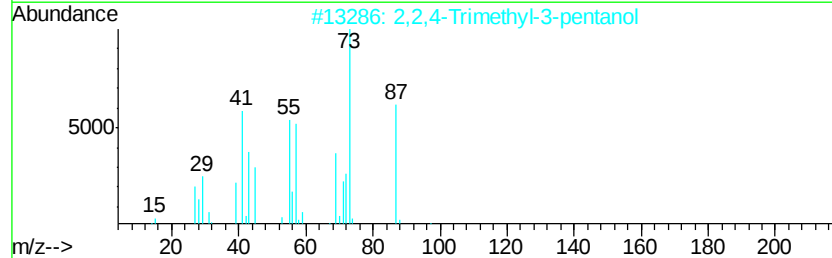
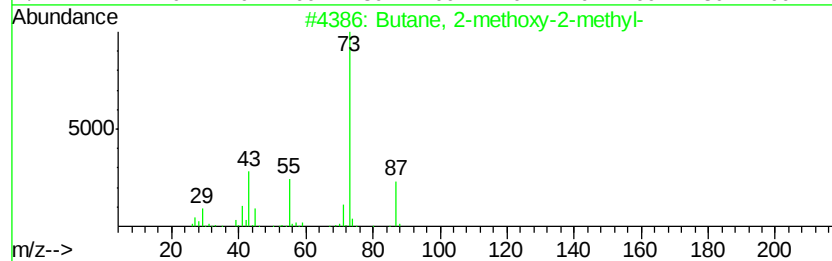
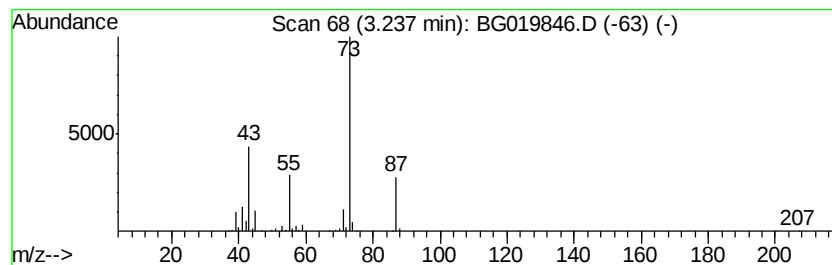
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.24	35.82 ng	246507	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Butanoic acid, 2-hydroxy-2-methyl...	132	C6H12O3	032793-34-3	23
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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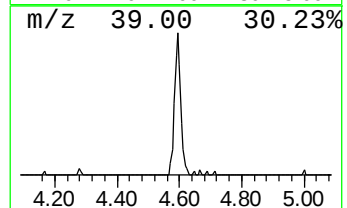
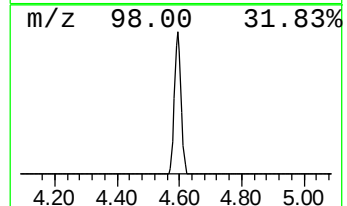
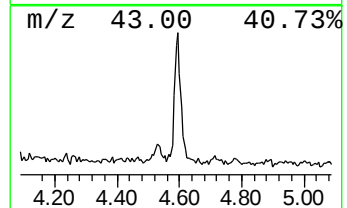
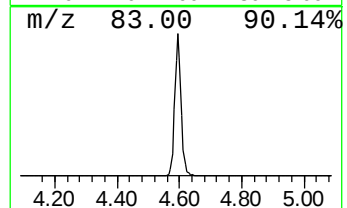
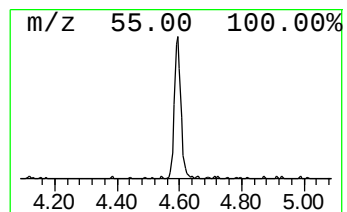
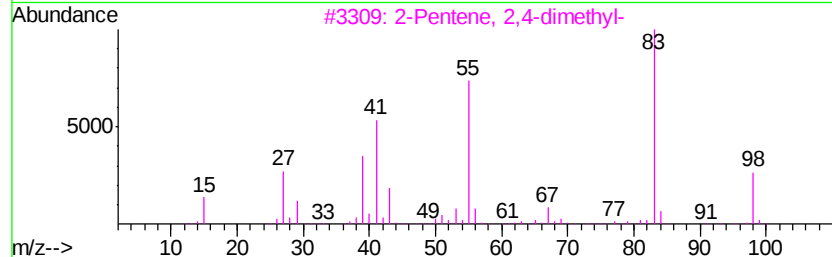
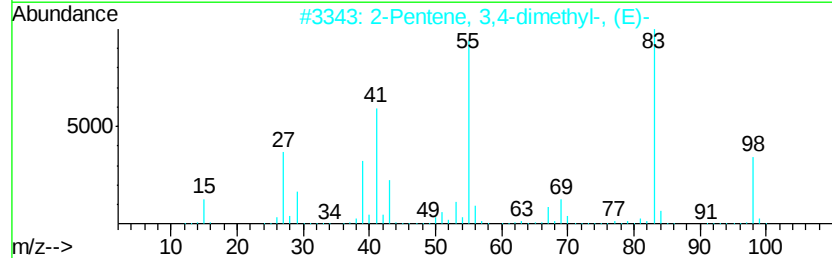
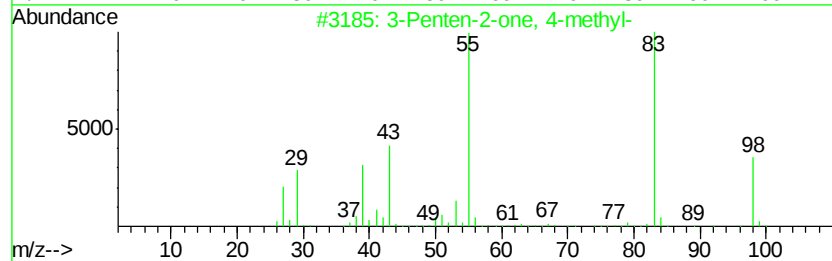
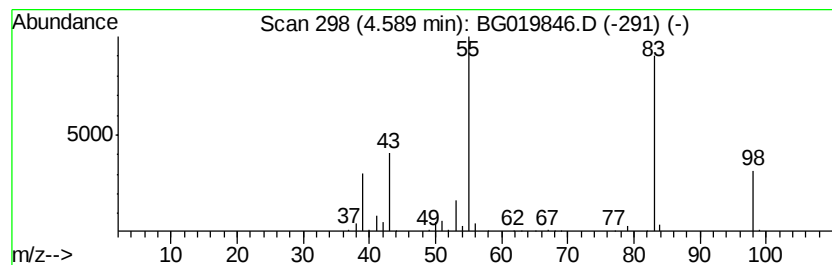
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Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	12.91 ng	88839	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		3-Hexen-2-one	98	C6H10O	000763-93-9	80
5		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	72



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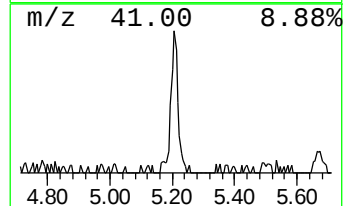
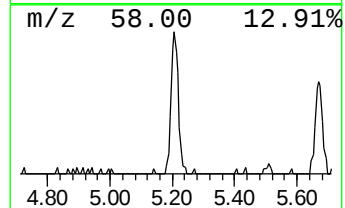
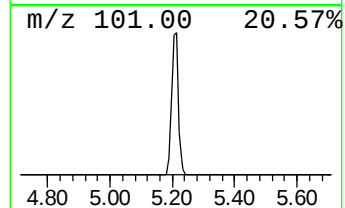
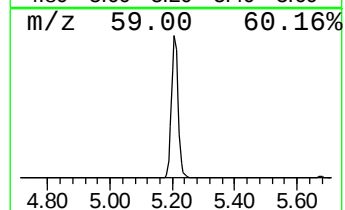
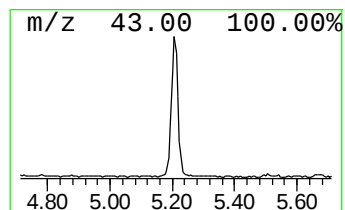
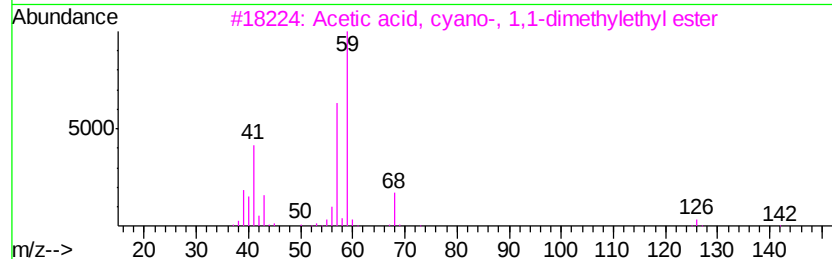
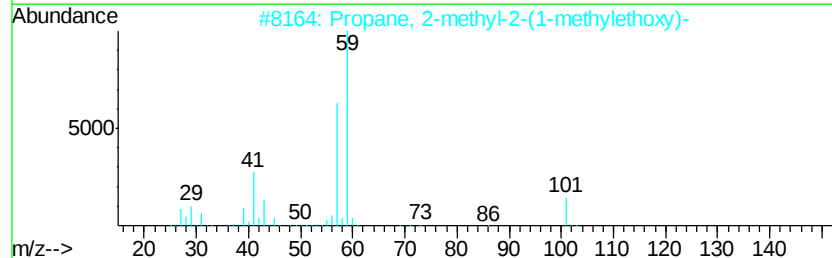
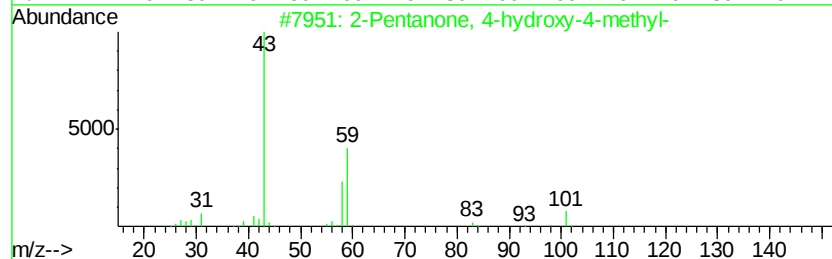
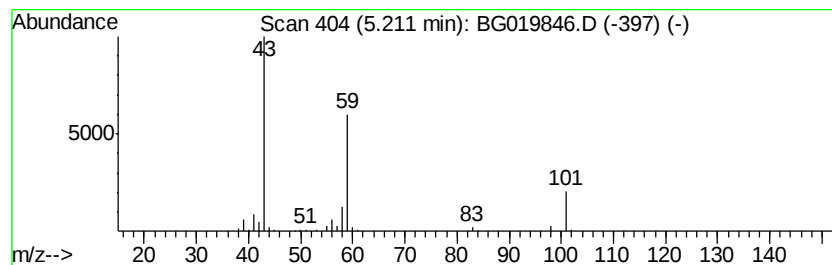
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	17.26 ng	118770	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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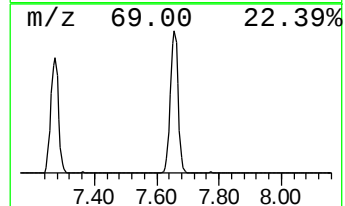
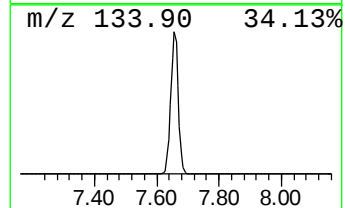
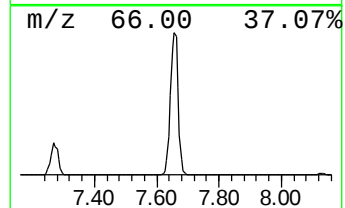
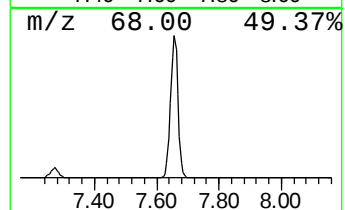
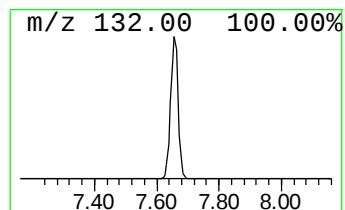
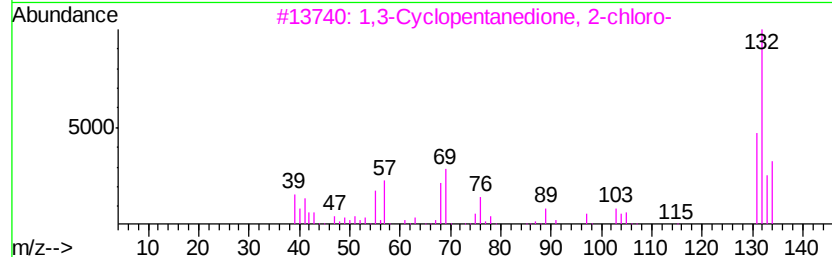
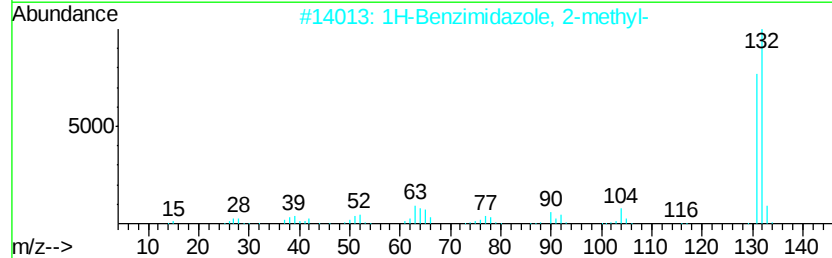
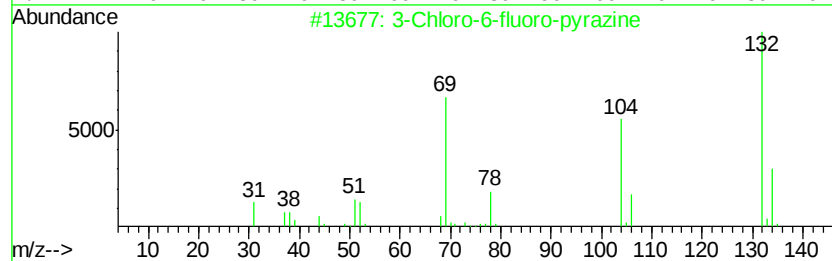
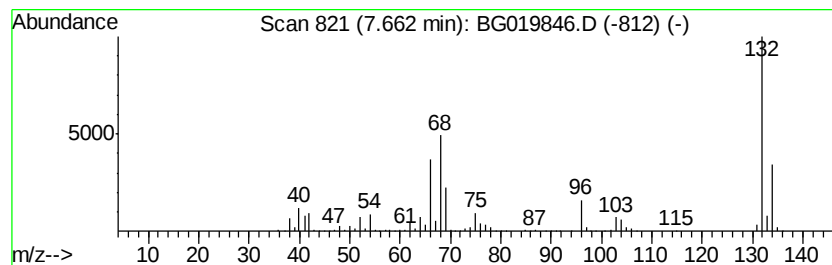
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	109.81 ng	755717	1,4-Dichlorobenzene-d4	8.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3			1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5			Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid	2.88	257.3	ng	1770590	1	8.13	137646	20.0
Butane, 2-methoxy...	3.24	35.8	ng	246507	1	8.13	137646	20.0
3-Penten-2-one, 4...	4.59	12.9	ng	88839	1	8.13	137646	20.0
2-Pentanone, 4-hy...	5.21	17.3	ng	118770	1	8.13	137646	20.0
unknown7.66	7.66	109.8	ng	755717	1	8.13	137646	20.0