

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120215\
Data File : BG019862.D
Acq On : 3 Dec 2015 9:34
Operator : UM/NP
Sample : G4583-13
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-P3WC-02(0-4)

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	2793827	1965123	66.11%	13.481%
2	3.144	46	52	63	rVV3	22910	56480	1.90%	0.387%
3	3.238	63	68	76	rVB	79319	115198	3.88%	0.790%
4	4.589	292	298	304	rBV2	59972	85649	2.88%	0.588%
5	5.206	397	403	410	rBV	123781	188714	6.35%	1.295%
6	5.670	475	482	490	rBV	486127	760458	25.58%	5.217%
7	7.268	746	754	763	rBV	476819	804945	27.08%	5.522%
8	7.656	812	820	828	rVB	518644	890041	29.94%	6.106%
9	8.126	893	900	907	rVB	86649	141724	4.77%	0.972%
10	8.449	947	955	963	rBV	395335	674223	22.68%	4.625%
11	9.295	1090	1099	1107	rVB	332036	594750	20.01%	4.080%
12	10.946	1373	1380	1385	rBV	116116	210253	7.07%	1.442%
13	10.993	1385	1388	1395	rVB	42358	67599	2.27%	0.464%
14	13.385	1787	1795	1803	rBV	1026951	1567673	52.74%	10.754%
15	14.759	2021	2029	2035	rBV2	203309	335536	11.29%	2.302%
16	16.240	2274	2281	2292	rBV	982751	1461845	49.18%	10.028%
17	17.497	2489	2495	2500	rBV2	311202	466679	15.70%	3.201%
18	17.897	2557	2563	2567	rBV	37716	53389	1.80%	0.366%
19	19.648	2857	2861	2868	rBV6	19323	30397	1.02%	0.209%
20	20.106	2932	2939	2946	rBV	2305139	2972377	100.00%	20.391%
21	21.781	3217	3224	3230	rBV	358374	604589	20.34%	4.148%
22	25.077	3776	3785	3795	rVB2	187533	529420	17.81%	3.632%

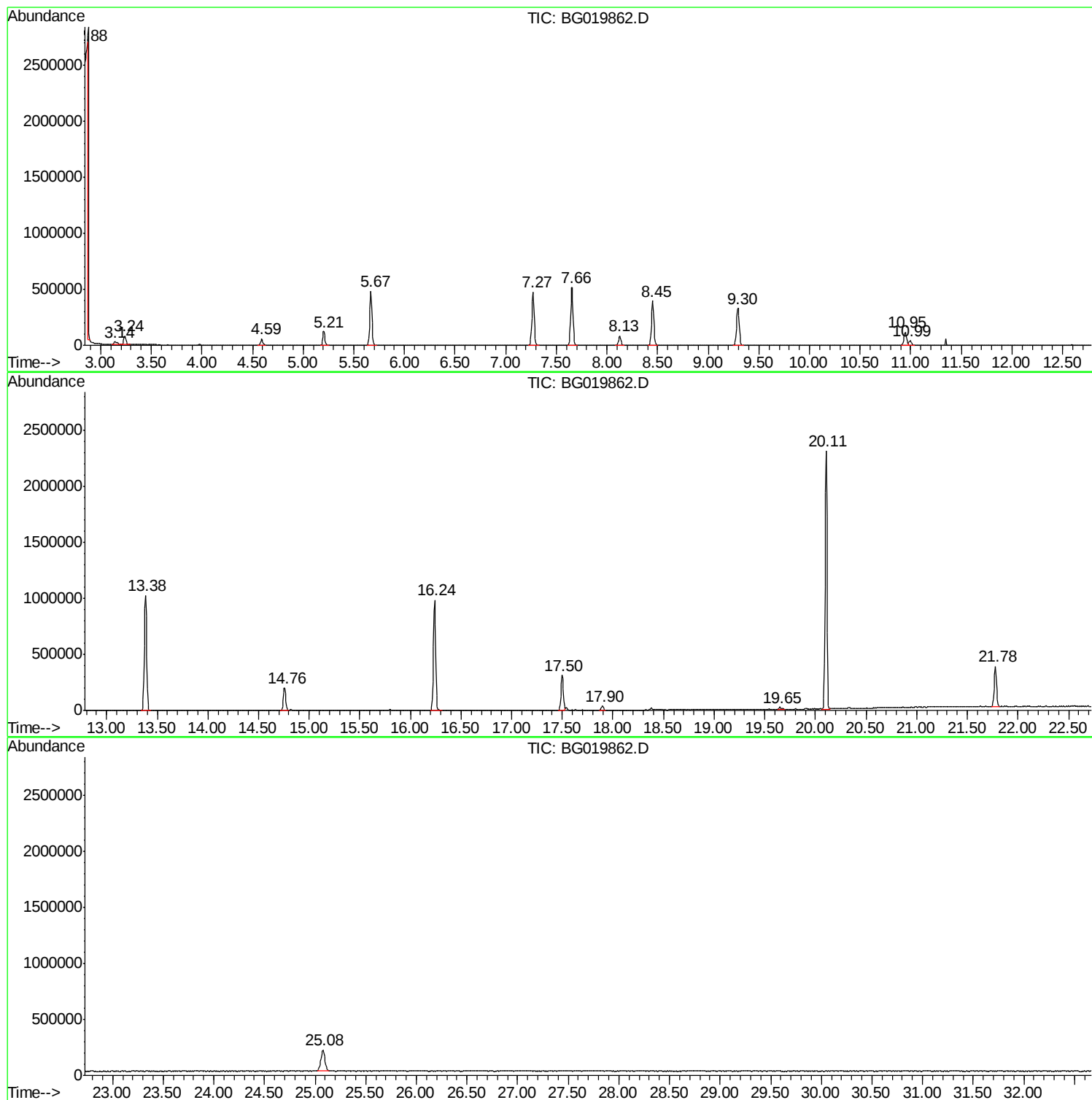
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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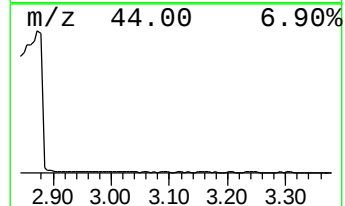
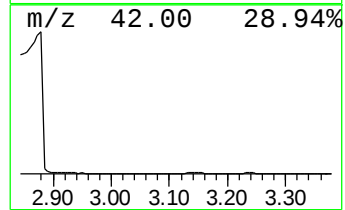
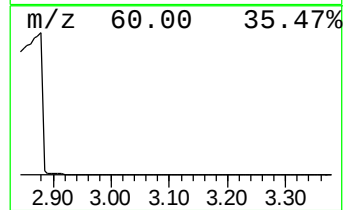
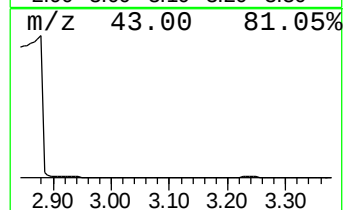
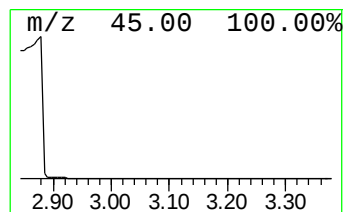
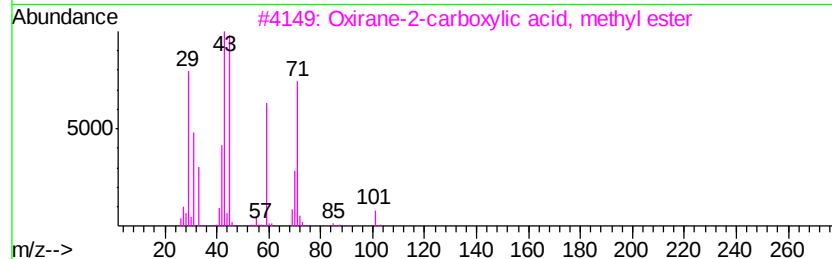
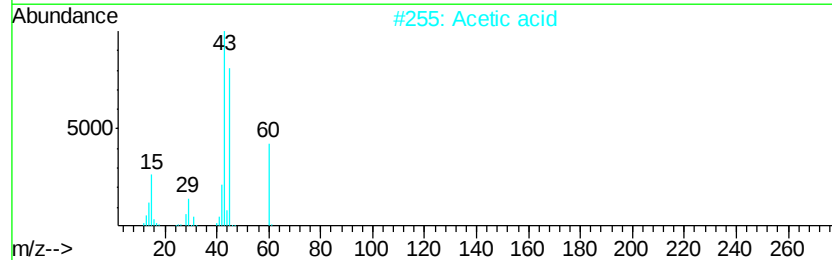
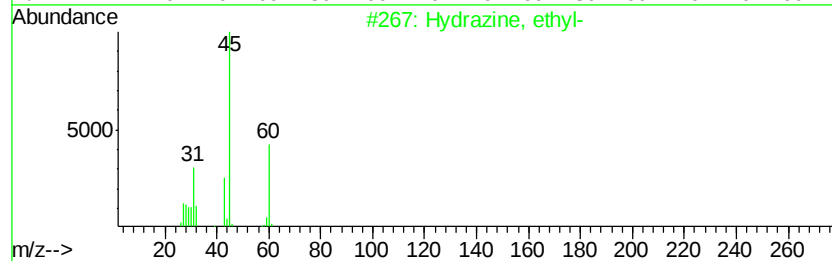
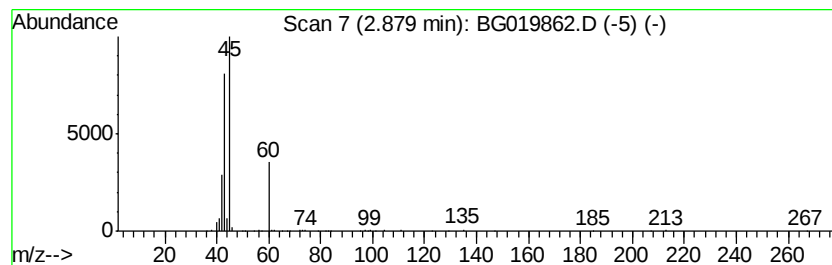
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.88 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	277.32 ng	1965120	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	42
2		Acetic acid	60	C2H4O2	000064-19-7	9
3		Oxirane-2-carboxylic acid, methy...	102	C4H6O3	004538-50-5	9
4		o-Acetyl-L-serine	147	C5H9NO4	005147-00-2	9
5		Methanamine, 1-methoxy-N-methyl-...	104	C3H8N2O2	039885-14-8	9



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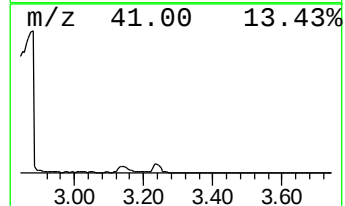
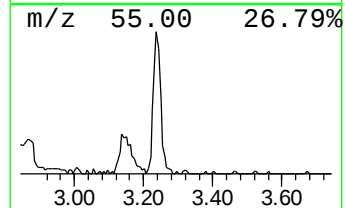
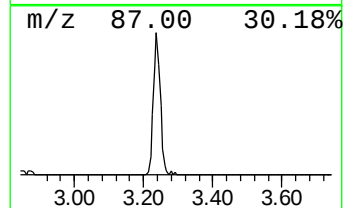
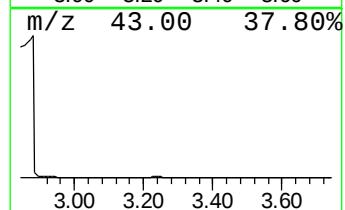
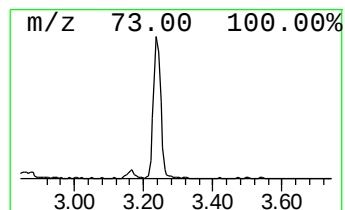
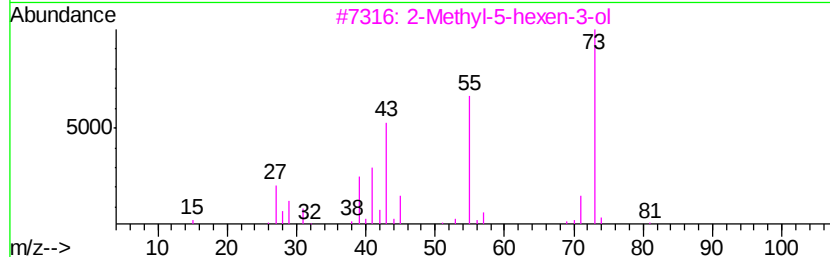
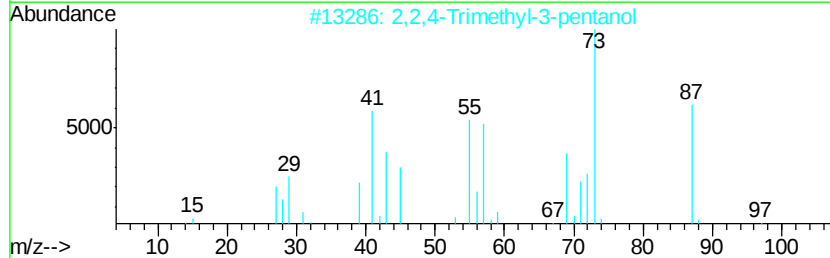
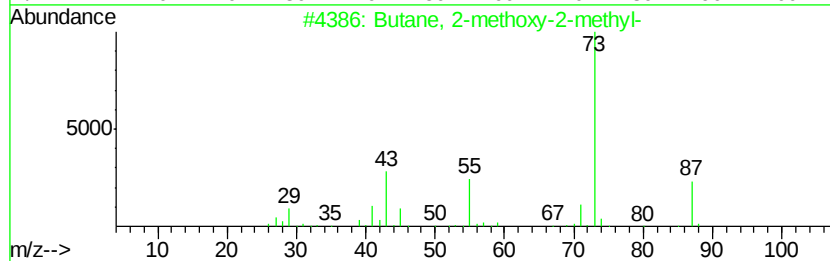
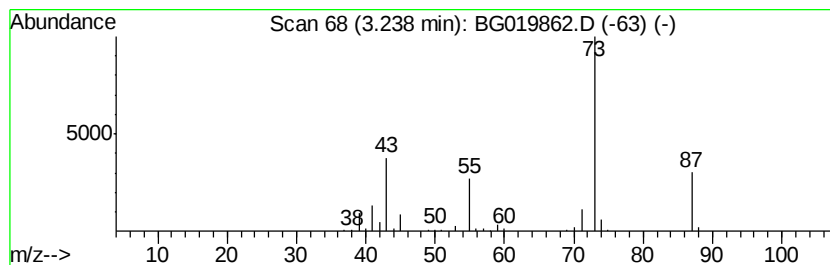
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.24	16.26 ng	115198	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	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12



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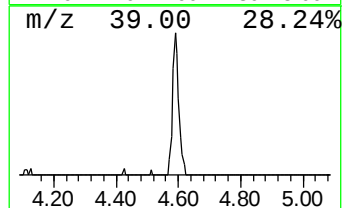
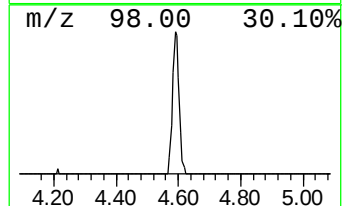
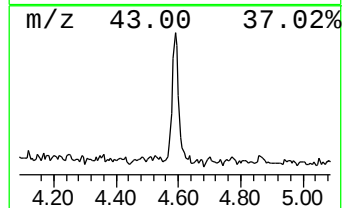
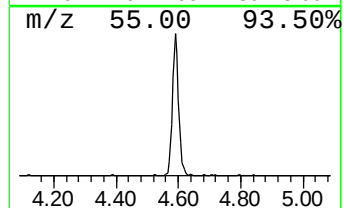
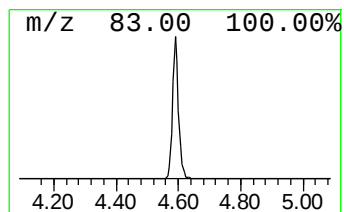
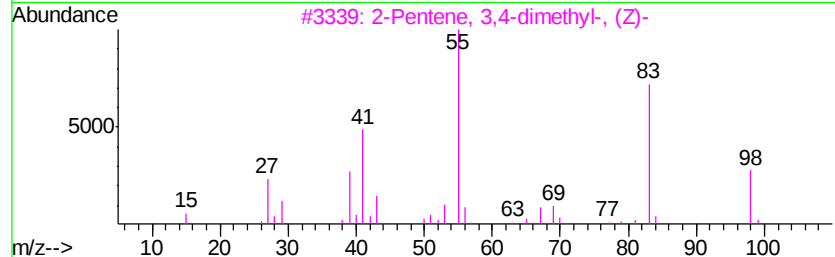
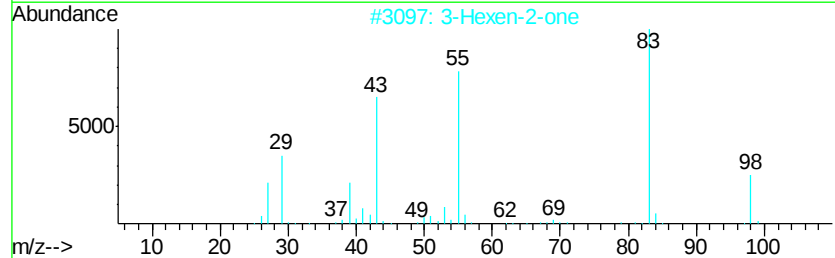
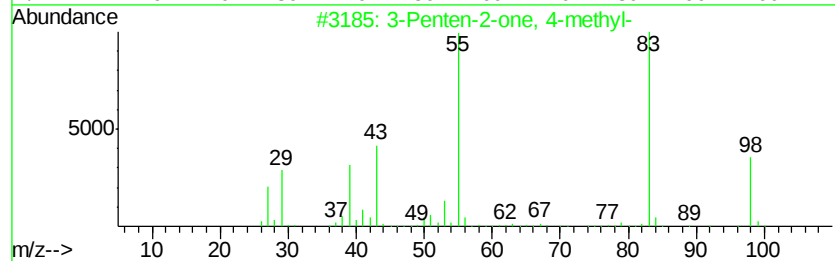
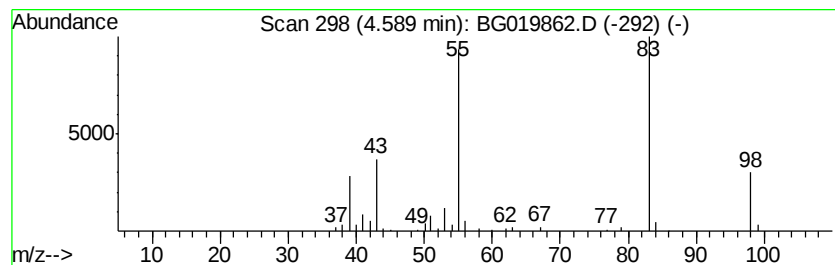
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	12.09 ng	85649	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	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86



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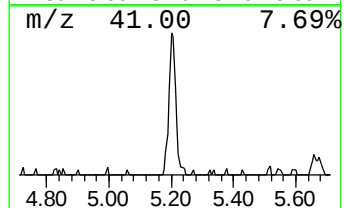
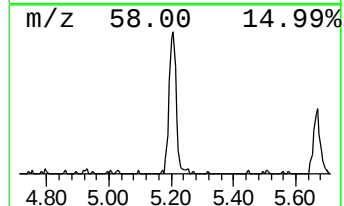
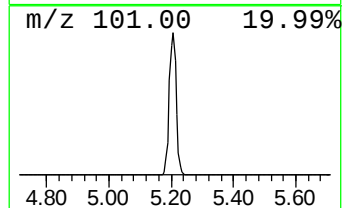
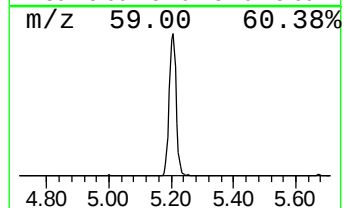
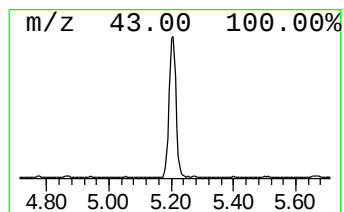
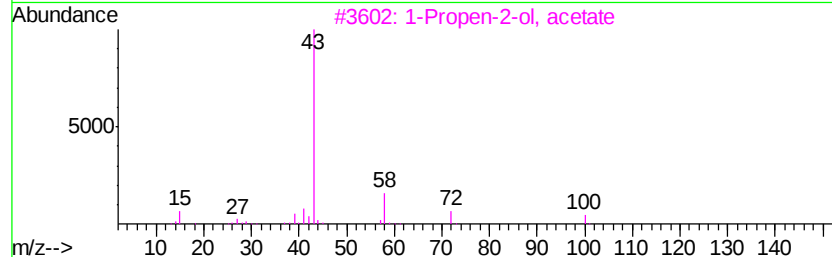
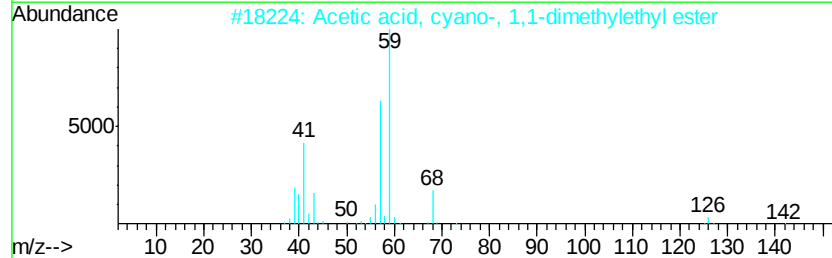
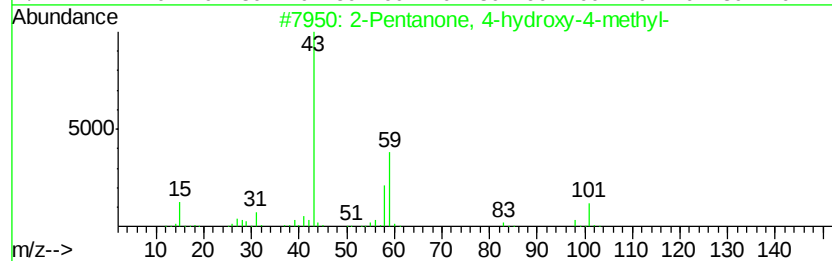
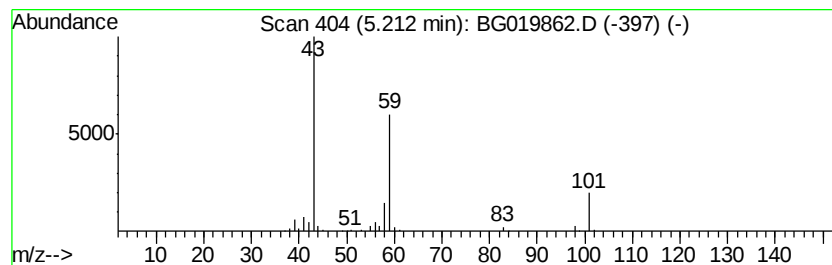
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	26.63 ng	188714	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		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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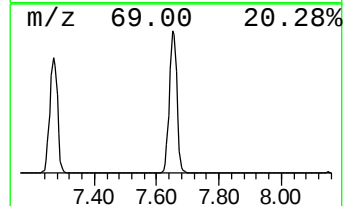
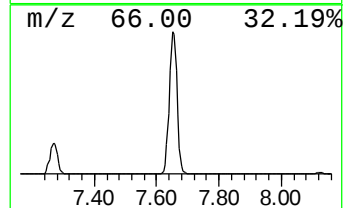
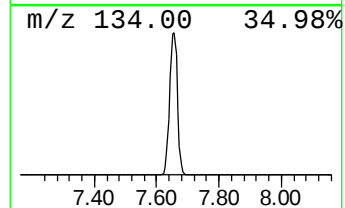
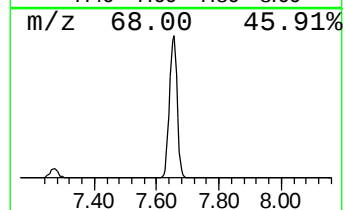
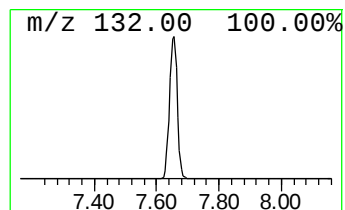
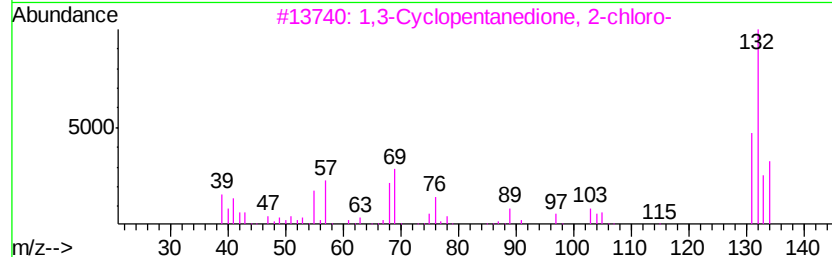
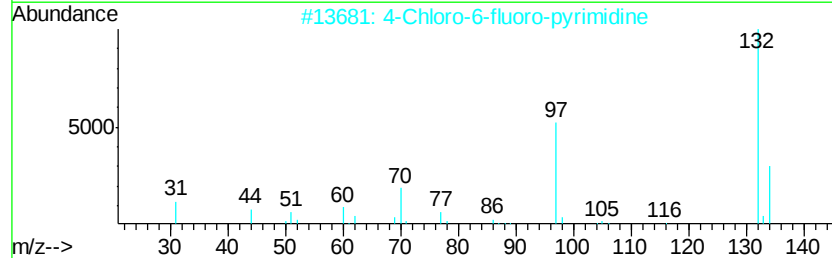
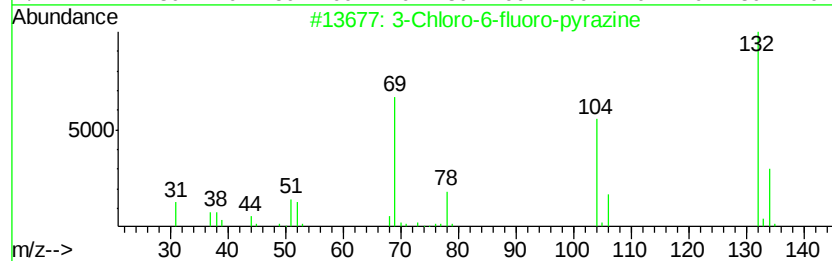
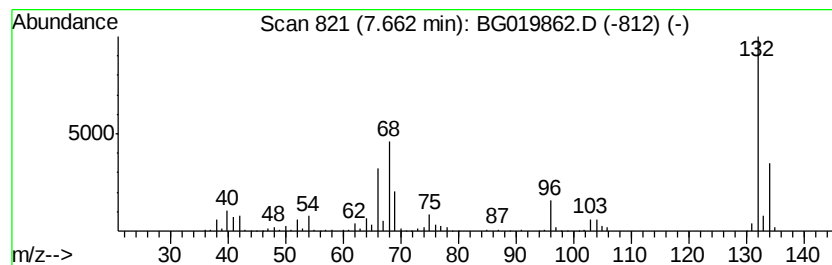
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Peak Number 6 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	125.60 ng	890041	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Benzene, 1-methyl-4-(1-methyleth...	132	C10H12	001195-32-0	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.88	2.88	277.3	ng	1965120	1	8.13	141724	20.0
Butane, 2-methoxy...	3.24	16.3	ng	115198	1	8.13	141724	20.0
3-Penten-2-one, 4...	4.59	12.1	ng	85649	1	8.13	141724	20.0
2-Pentanone, 4-hy...	5.21	26.6	ng	188714	1	8.13	141724	20.0
unknown7.66	7.66	125.6	ng	890041	1	8.13	141724	20.0