

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050316\
 Data File : BF086660.D
 Acq On : 3 May 2016 23:57
 Operator : UM/SJ
 Sample : H2716-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 26WARD-3-CS-4(0-12FTBGS)

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_F\METHODS\8270-BF042716.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	2.521	36	38	50	rVB	111733	204867	2.38%	0.415%
2	3.253	98	102	108	rBV	134760	279317	3.24%	0.566%
3	4.281	187	192	194	rBV	4777811	8621855	100.00%	17.470%
4	4.933	247	249	257	rBV	746173	1208118	14.01%	2.448%
5	5.356	283	286	289	rBV	4021464	4766204	55.28%	9.658%
6	6.396	374	377	380	rBV	3894048	4458914	51.72%	9.035%
7	6.522	386	388	391	rBV	4857987	4854107	56.30%	9.836%
8	6.750	406	408	415	rBV	1174808	1156313	13.41%	2.343%
9	6.910	419	422	424	rBV	4200647	3884641	45.06%	7.871%
10	7.322	455	458	460	rBV	3349124	3444478	39.95%	6.979%
11	8.042	518	521	530	rBV	1125057	1564806	18.15%	3.171%
12	9.116	612	615	618	rBV	5074063	4747020	55.06%	9.619%
13	9.790	671	674	676	rBV	1457372	1347742	15.63%	2.731%
14	10.579	740	743	745	rBV	2290115	2683731	31.13%	5.438%
15	11.265	801	803	813	rBV	999590	1025750	11.90%	2.078%
16	12.854	939	942	945	rBV	3647790	3513198	40.75%	7.119%
17	13.894	1031	1033	1041	rBV	745052	921846	10.69%	1.868%
18	15.288	1152	1155	1158	rBV	513466	669019	7.76%	1.356%

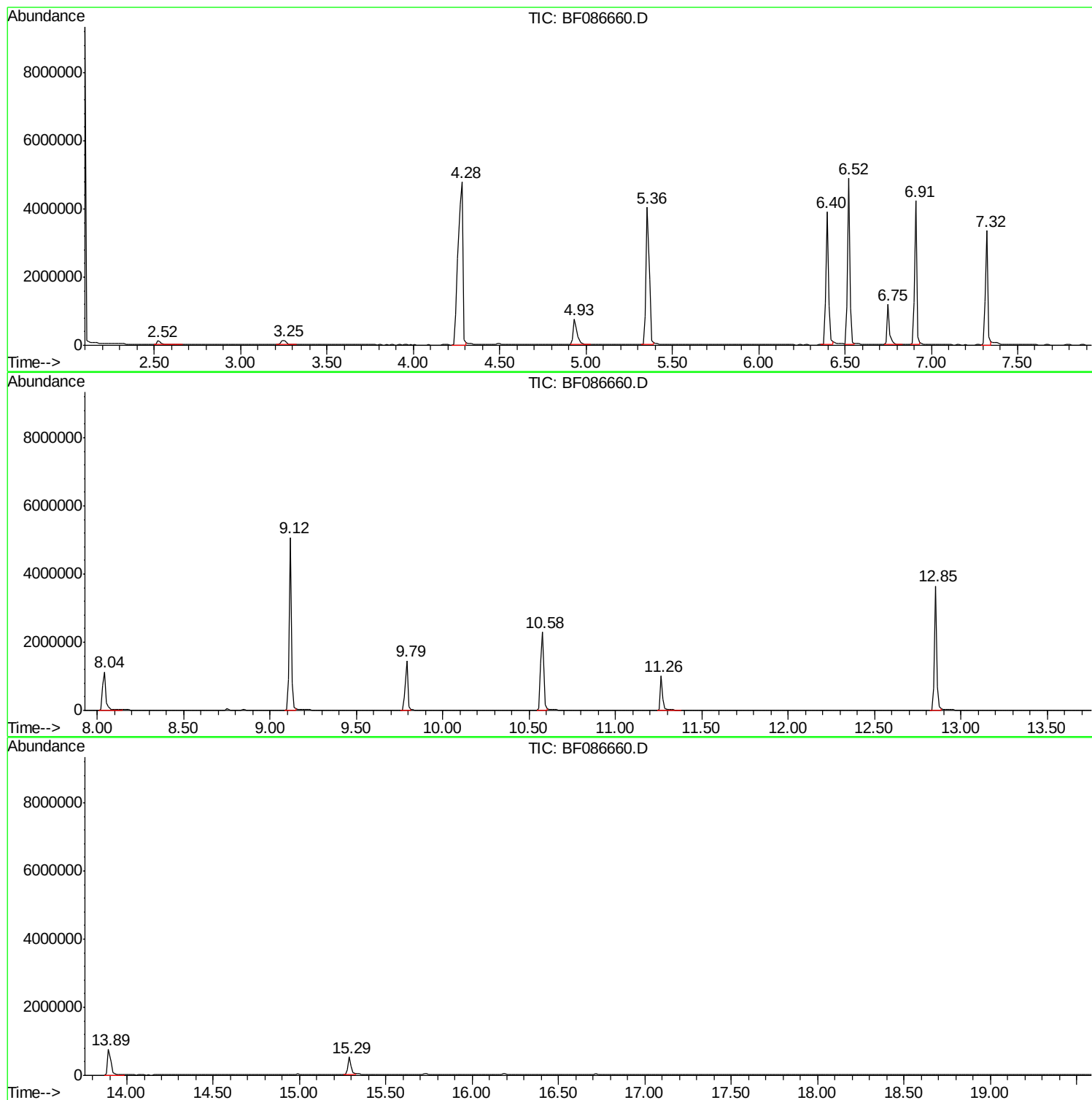
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Data Path : Z:\HPCHEM1\BNA_F\DATA\BF050316\
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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
26WARD-3-CS-4(0-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.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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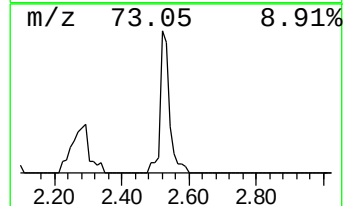
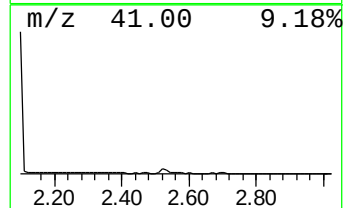
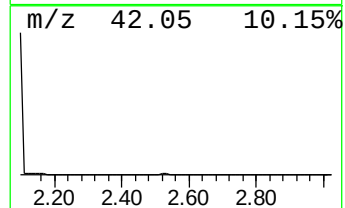
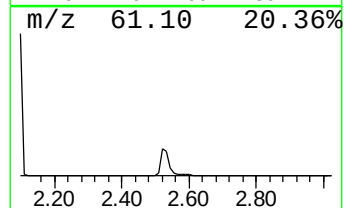
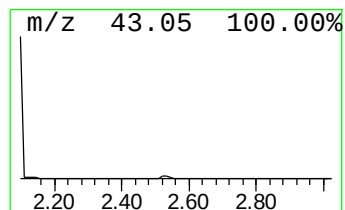
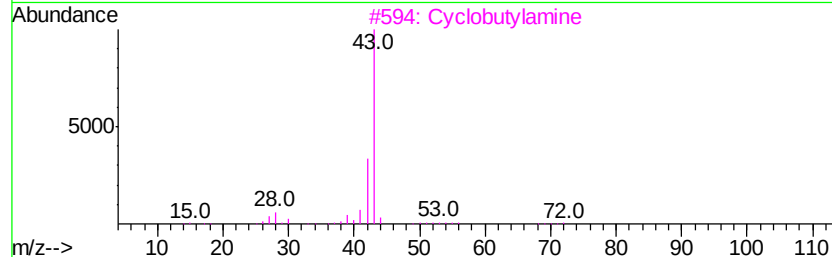
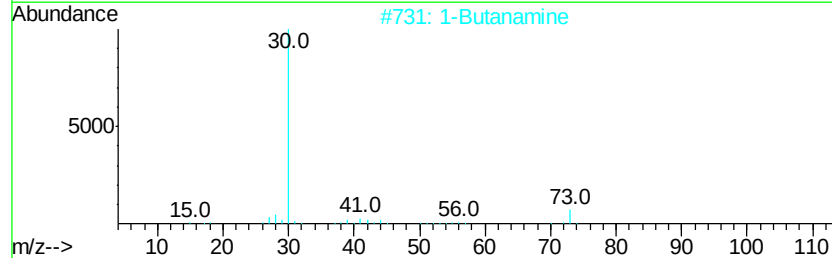
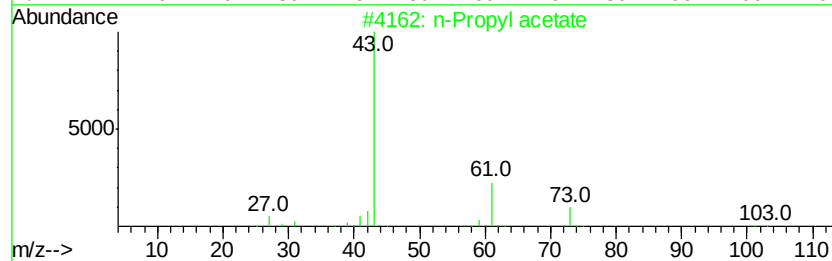
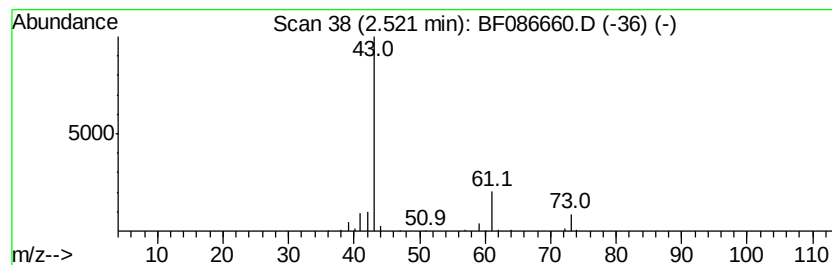
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ClientSampleId :
26WARD-3-CS-4(0-12FTBGS)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
2.52	3.54 ng	204867	1,4-Dichlorobenzene-d4		6.75
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Cyclobutylamine	71	C4H9N	002516-34-9	4
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4
5	Hydrogen azide	43	HN3	007782-79-8	4



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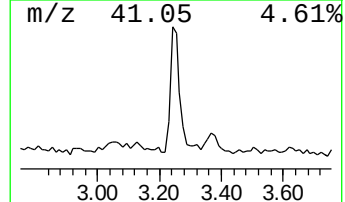
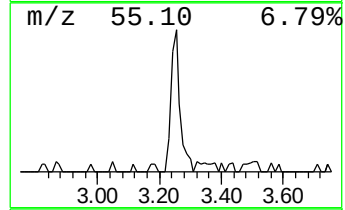
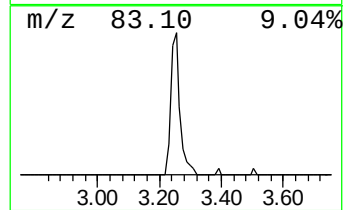
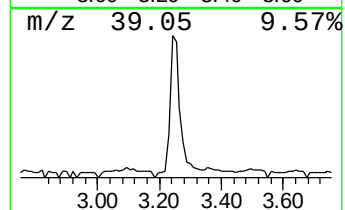
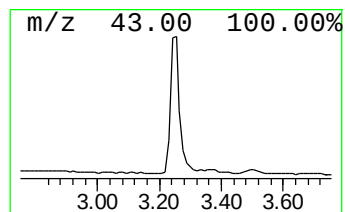
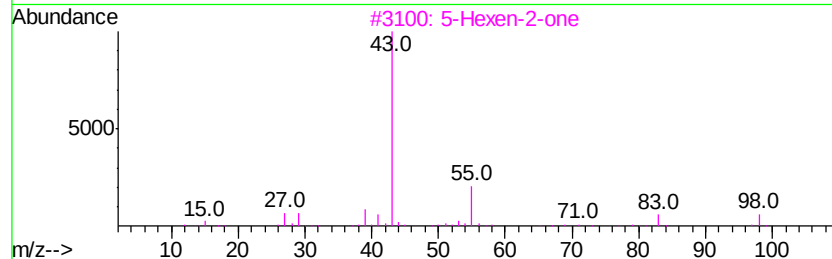
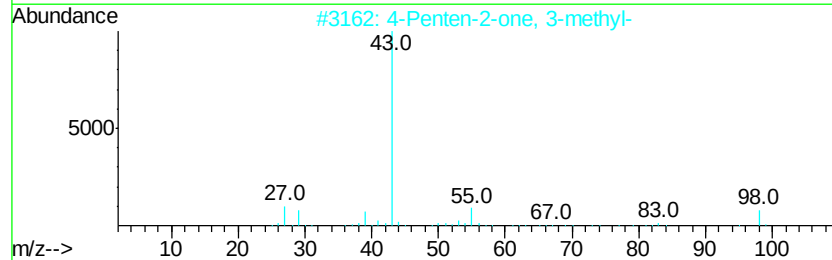
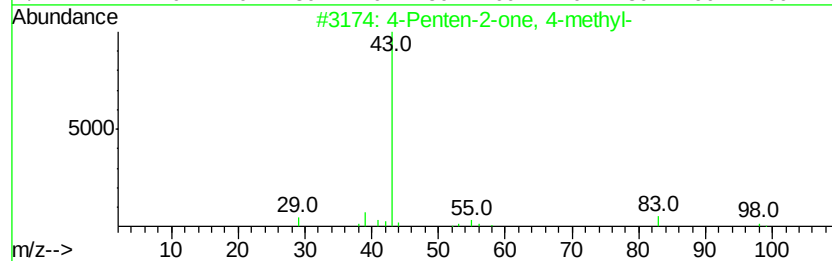
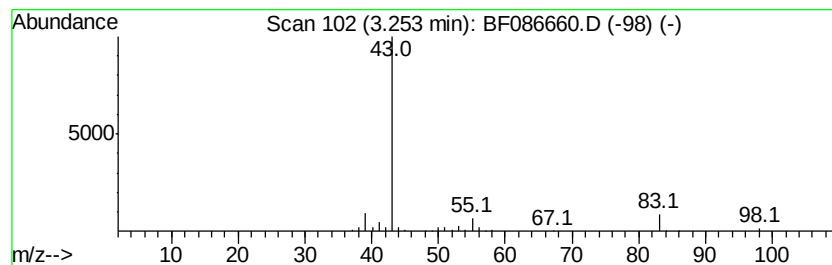
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.25	4.83 ng	279317	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	80
2		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	53
3		5-Hexen-2-one	98	C6H10O	000109-49-9	40
4		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	30
5		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	17



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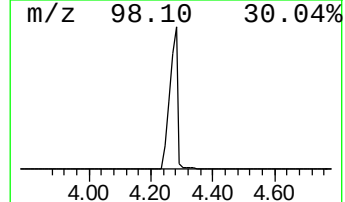
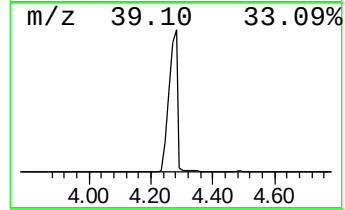
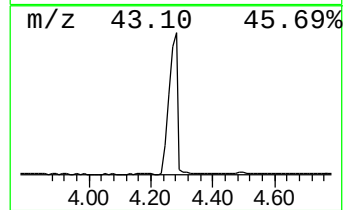
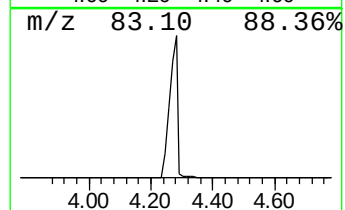
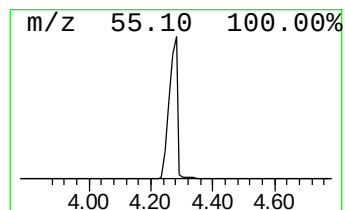
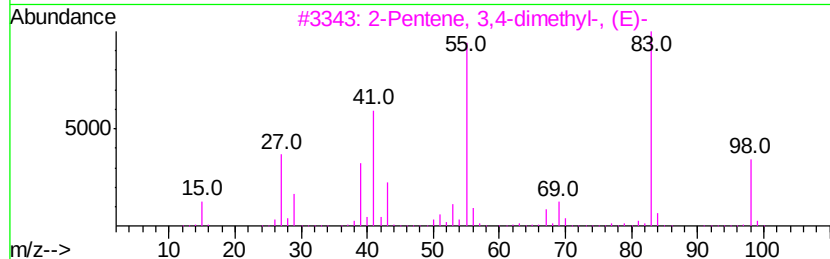
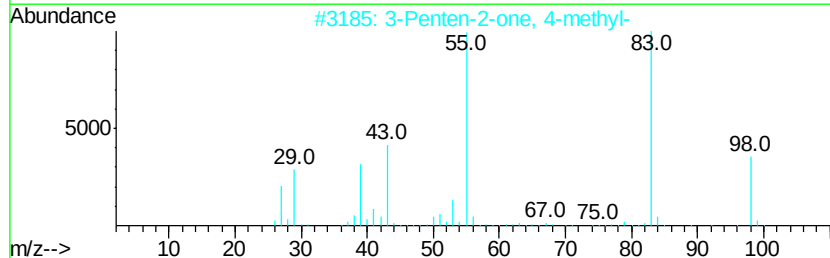
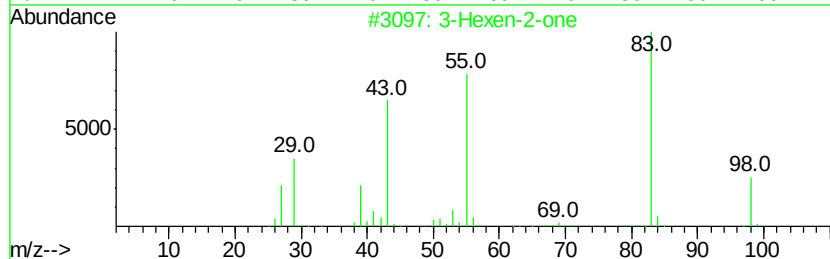
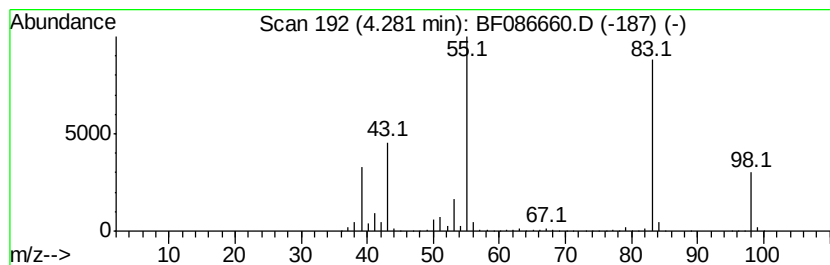
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Peak Number 3 3-Hexen-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.28	149.13 ng	8621860	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78



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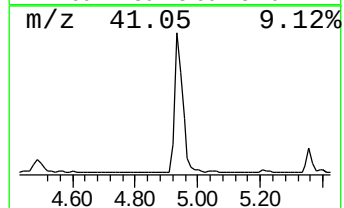
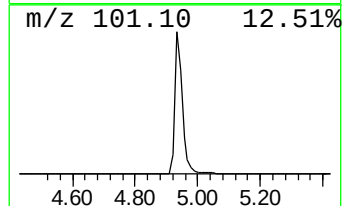
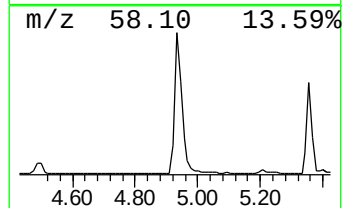
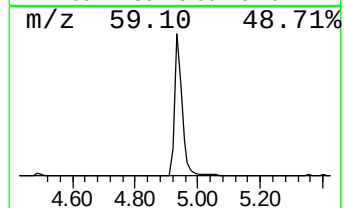
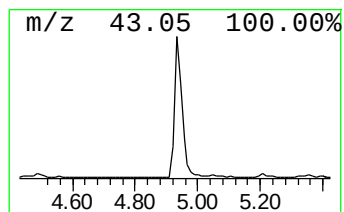
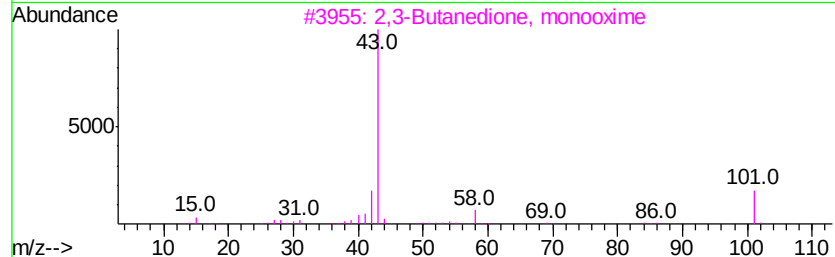
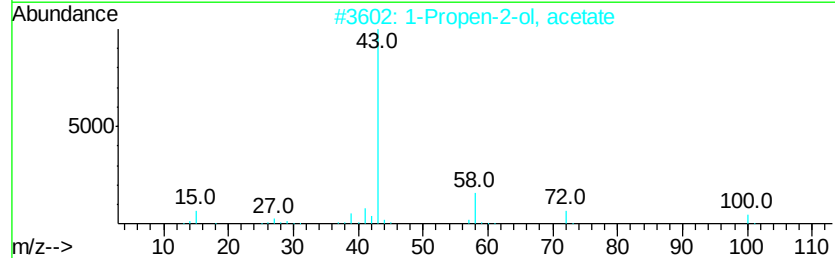
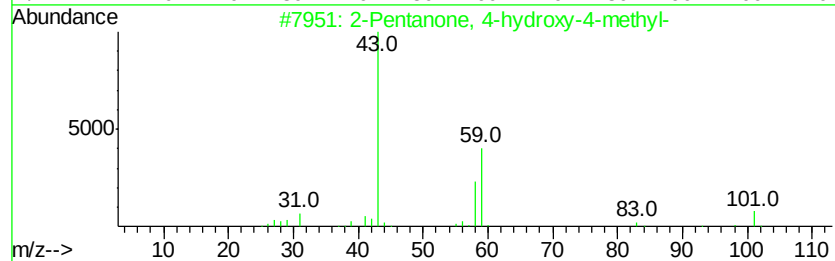
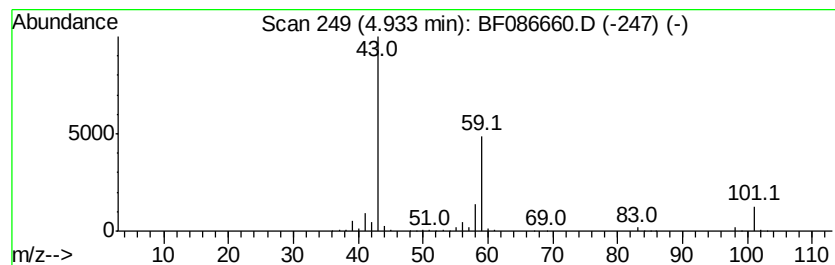
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	20.90 ng	1208120	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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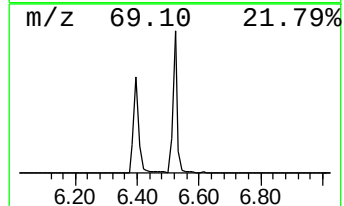
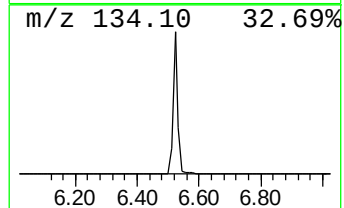
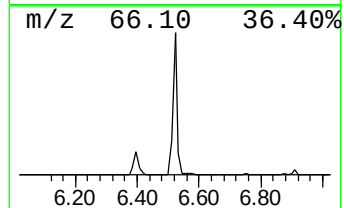
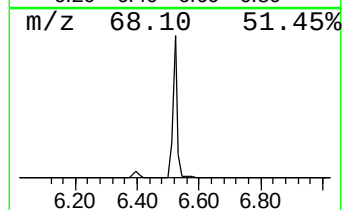
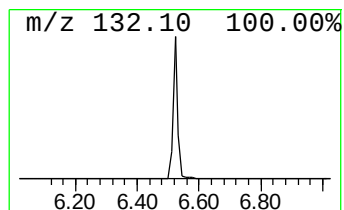
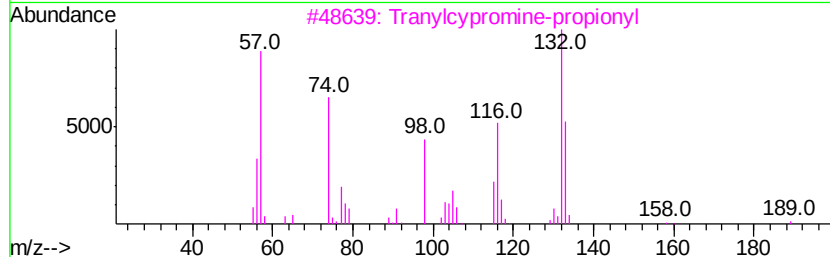
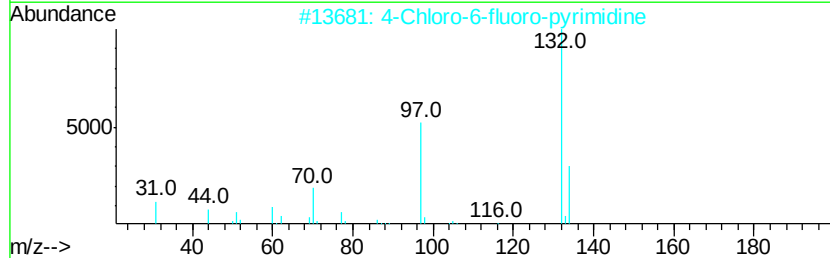
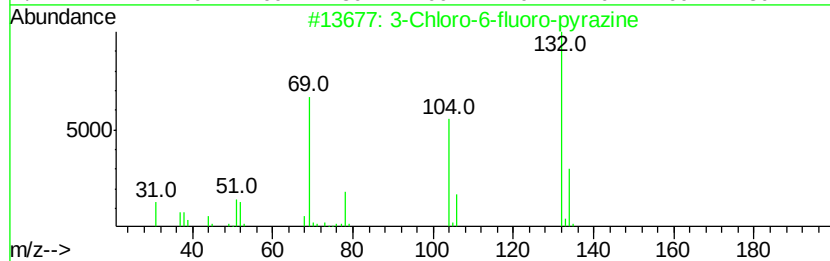
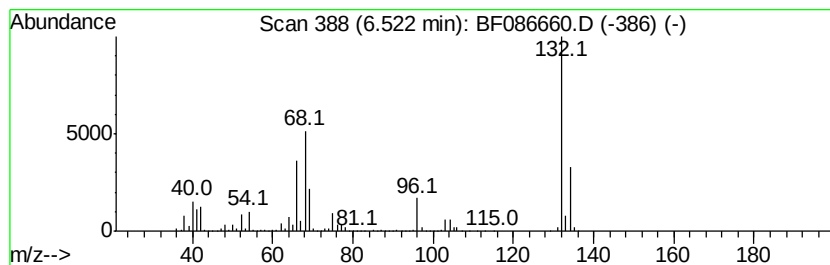
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Peak Number 5 unknown6.52 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	83.96 ng	4854110	1,4-Dichlorobenzene-d4	6.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine			132	C4H2ClFN2	051422-01-6	27
3	Tranvlcvpromine-propionyl			189	C12H15NO	1000123-86-3	22
4	Pyrazolo(2,3-a)pyridine, 7-methyl-			132	C8H8N2	034760-58-2	22
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
n-Propyl acetate	2.52	3.5	ng	204867	1	6.75	1156310	20.0
4-Penten-2-one, 4...	3.25	4.8	ng	279317	1	6.75	1156310	20.0
3-Hexen-2-one	4.28	149.1	ng	8621860	1	6.75	1156310	20.0
2-Pentanone, 4-hy...	4.93	20.9	ng	1208120	1	6.75	1156310	20.0
unknown6.52	6.52	84.0	ng	4854110	1	6.75	1156310	20.0