

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111414\
 Data File : BF075505.D
 Acq On : 14 Nov 2014 20:34
 Operator : TP / JJ
 Sample : PB80189BL
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB80189BL

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-BF111214.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	1.624	45	47	50	rVB	315141	326273	17.59%	2.472%
2	1.761	55	59	63	rVB	35991	79448	4.28%	0.602%
3	1.830	63	65	70	rBV	25558	37634	2.03%	0.285%
4	1.967	75	77	85	rBV	143559	213405	11.50%	1.617%
5	4.573	302	305	312	rVB	172030	228530	12.32%	1.731%
6	5.350	370	373	376	rBV	1584710	1854996	100.00%	14.052%
7	5.841	413	416	418	rBV	785962	813319	43.84%	6.161%
8	6.344	458	460	462	rBV	67355	65426	3.53%	0.496%
9	7.087	523	525	528	rBV	813013	785311	42.33%	5.949%
10	7.259	537	540	542	rBV	883951	826565	44.56%	6.261%
11	7.544	563	565	568	rVB	222213	297259	16.02%	2.252%
12	7.739	580	582	584	rVB	1127322	1012476	54.58%	7.670%
13	8.242	623	626	628	rVB	825583	788753	42.52%	5.975%
14	9.133	702	704	706	rBV	417387	423479	22.83%	3.208%
15	10.470	819	821	824	rBV	1189980	1435580	77.39%	10.875%
16	11.305	892	894	897	rBV	361206	443376	23.90%	3.359%
17	12.288	978	980	983	rBV	553025	530902	28.62%	4.022%
18	13.156	1054	1056	1059	rVB	462344	443305	23.90%	3.358%
19	15.157	1228	1231	1233	rBV	1412508	1595743	86.02%	12.088%
20	16.448	1342	1344	1347	rBV	450198	491933	26.52%	3.727%
21	18.197	1494	1497	1500	rBV	364324	507167	27.34%	3.842%

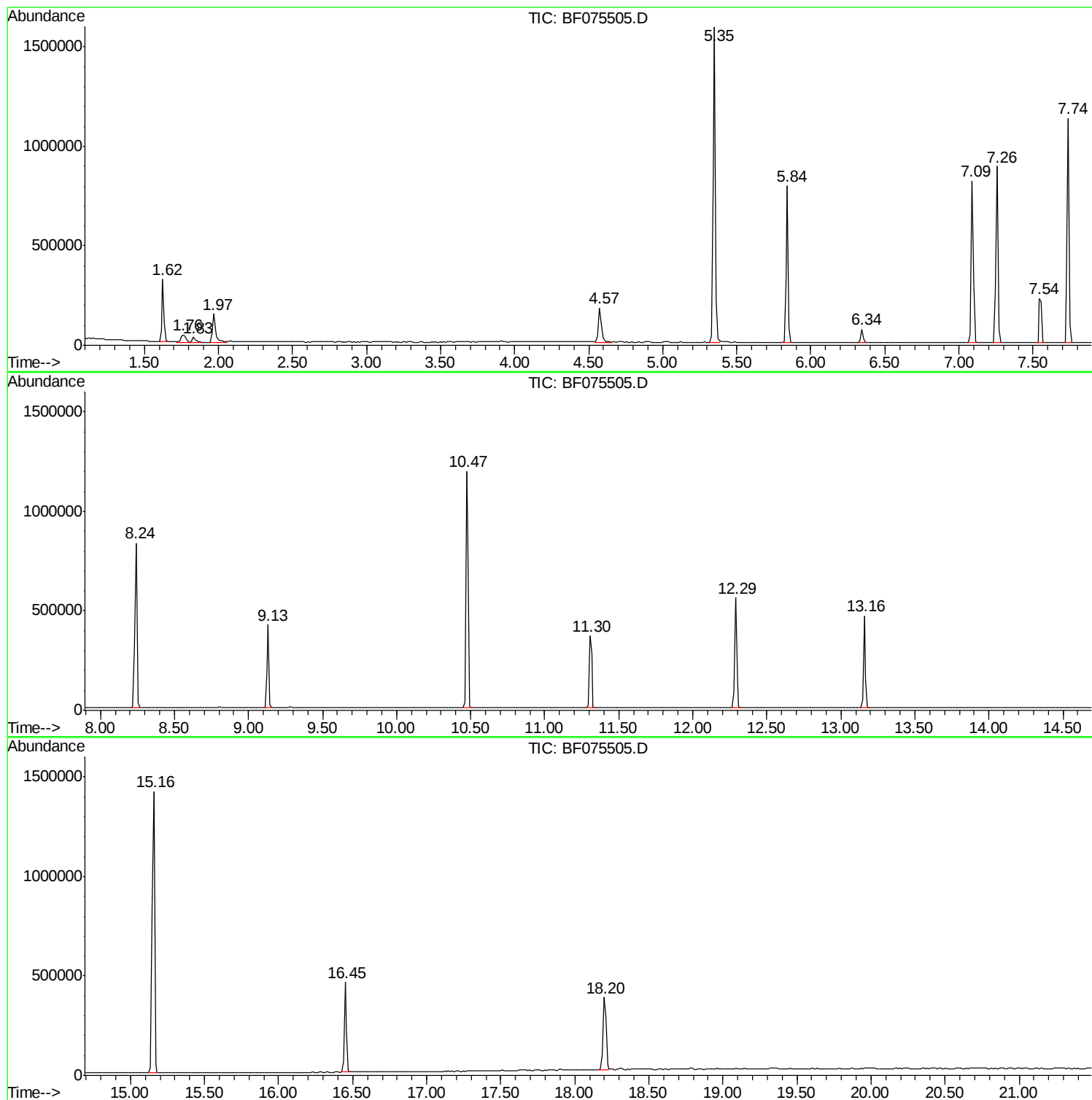
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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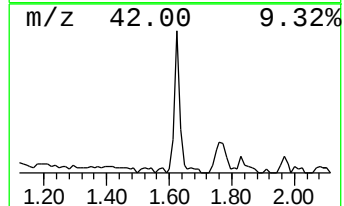
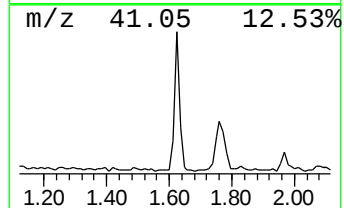
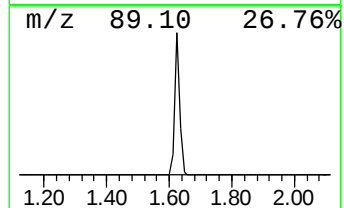
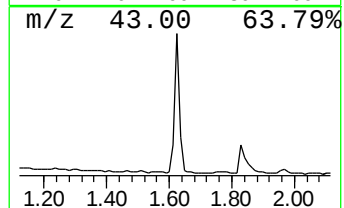
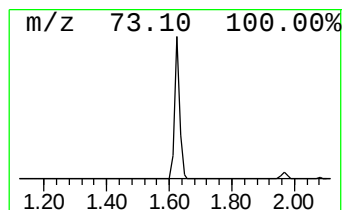
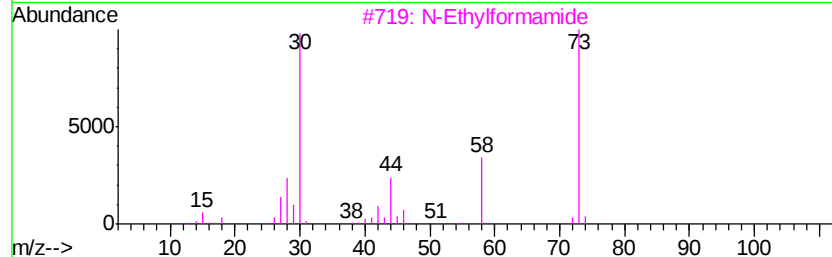
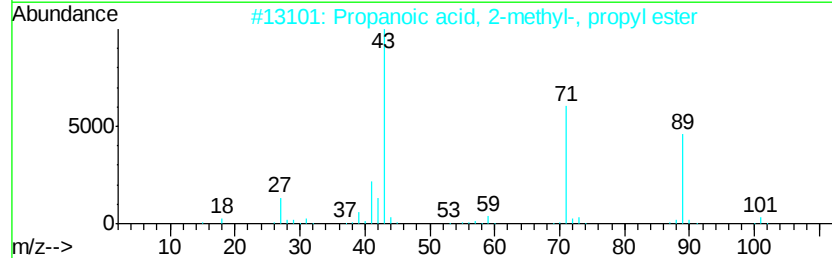
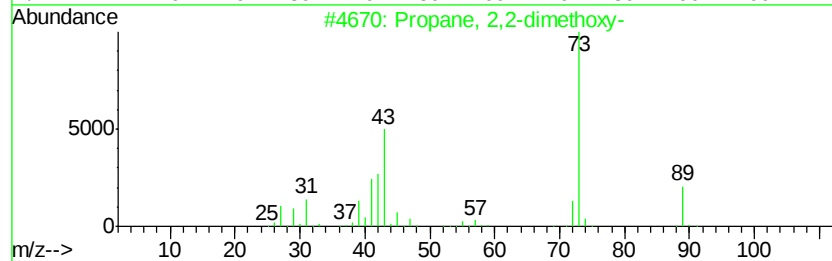
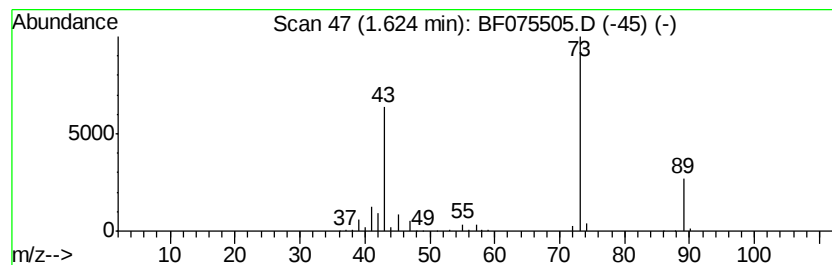
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.62	21.95 ng	326273	1,4-Dichlorobenzene-d4	7.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2			Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	25
3			N-Ethylformamide	73	C3H7NO	000627-45-2	9
4			1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
5			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9



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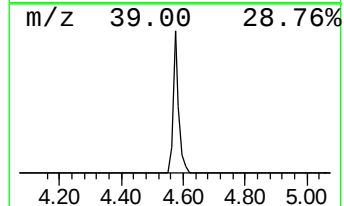
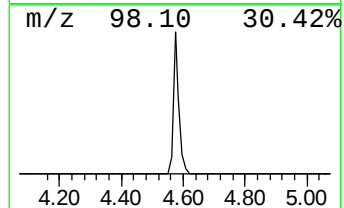
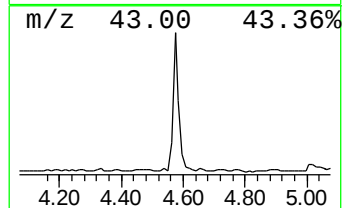
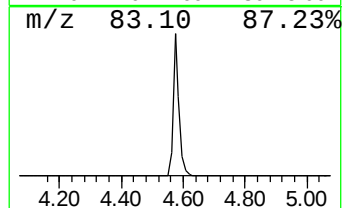
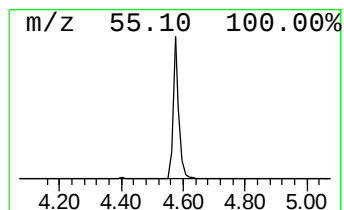
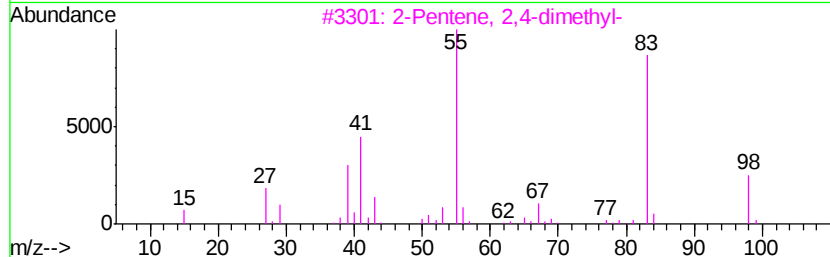
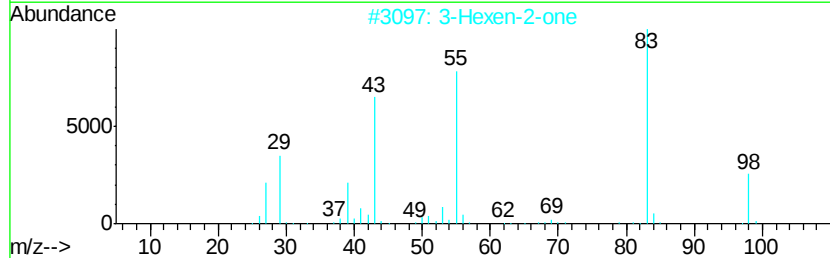
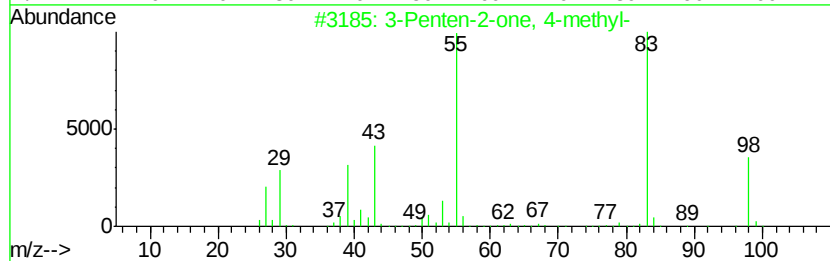
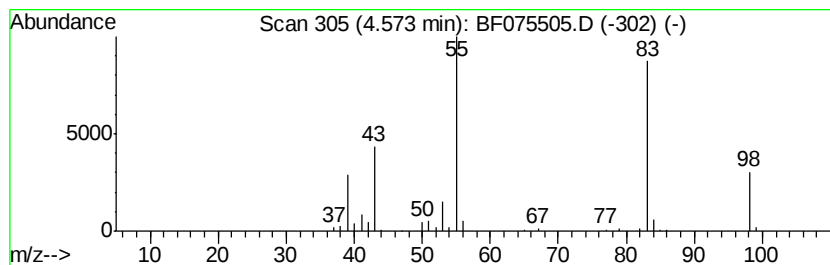
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	15.38 ng	228530	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	87
3		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80
5		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	80



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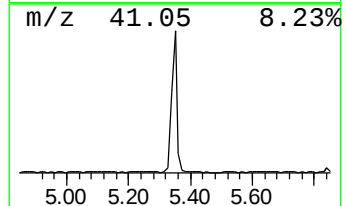
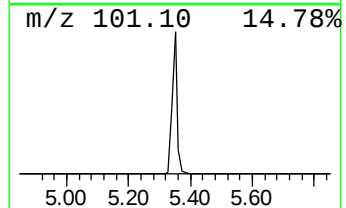
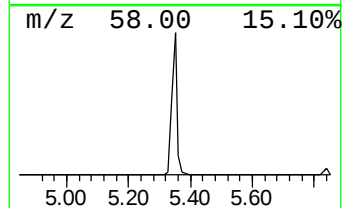
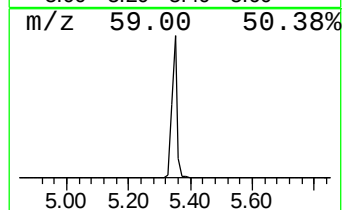
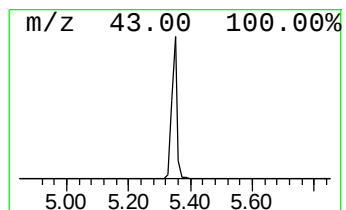
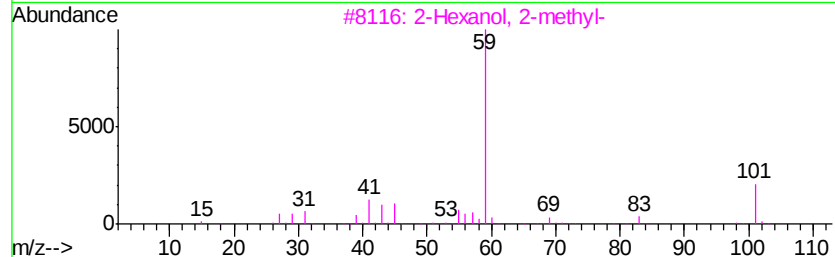
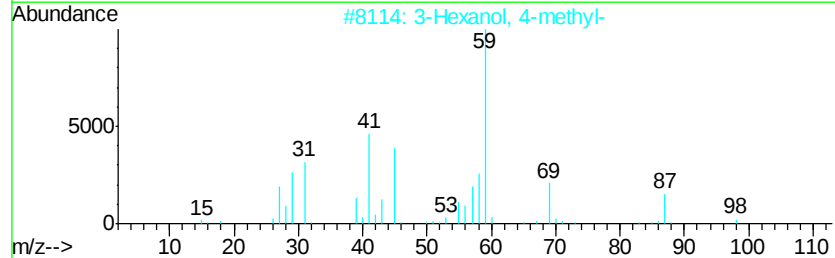
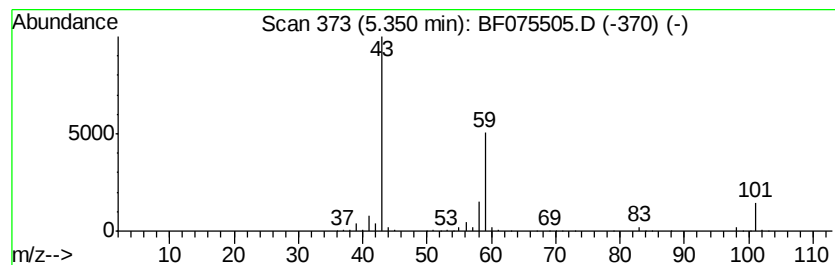
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.35	124.81 ng	1855000	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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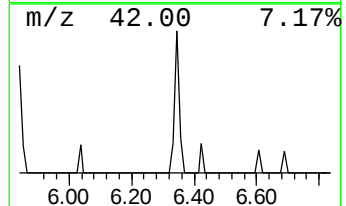
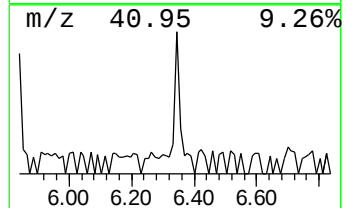
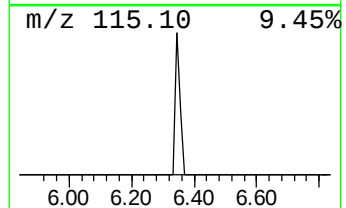
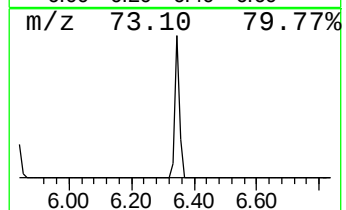
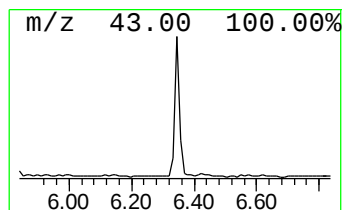
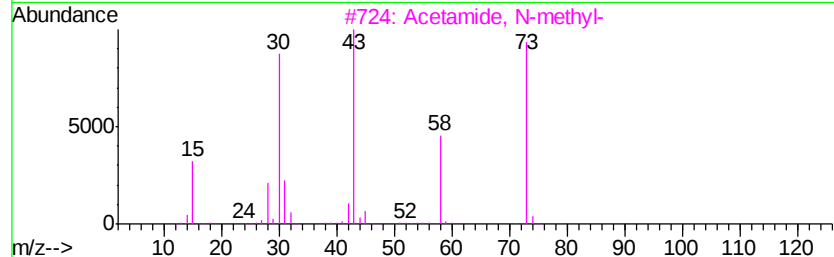
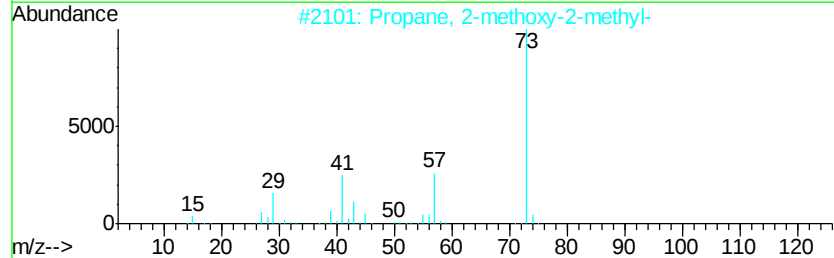
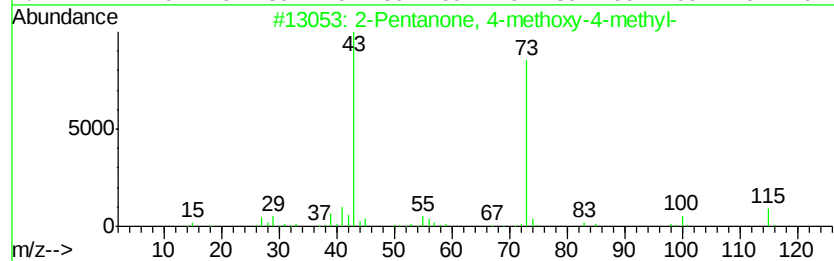
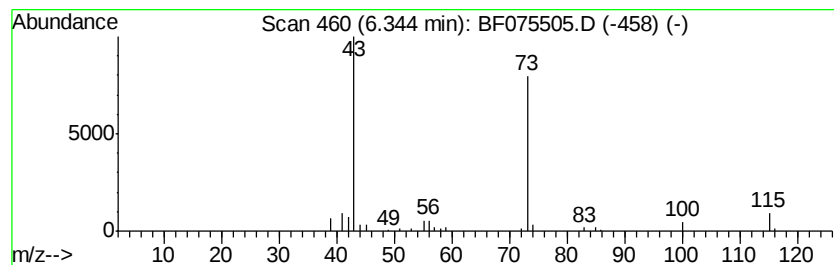
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Propane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	4.40 ng	65426	1,4-Dichlorobenzene-d4	7.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4		N-Formylmorpholine	115	C5H9NO2	004394-85-8	9
5		1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	9



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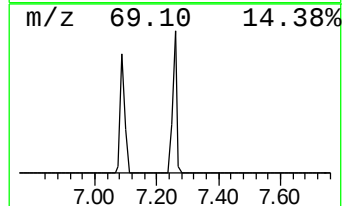
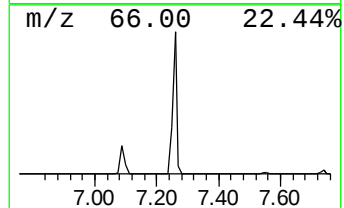
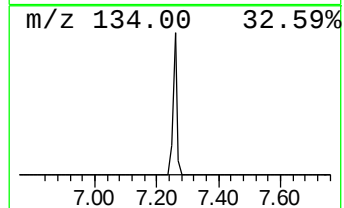
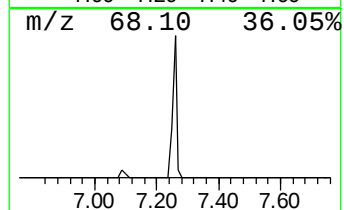
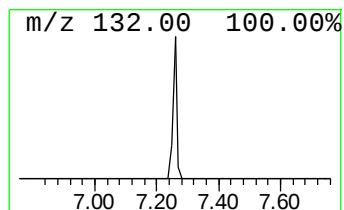
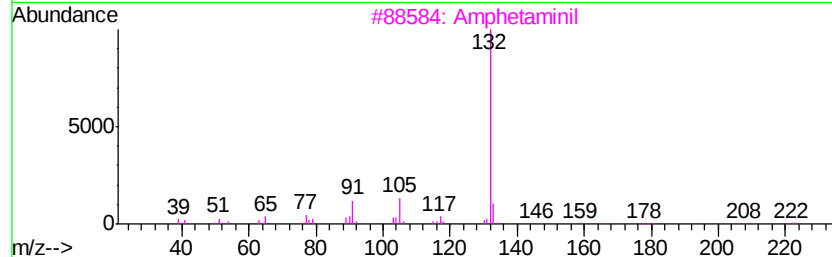
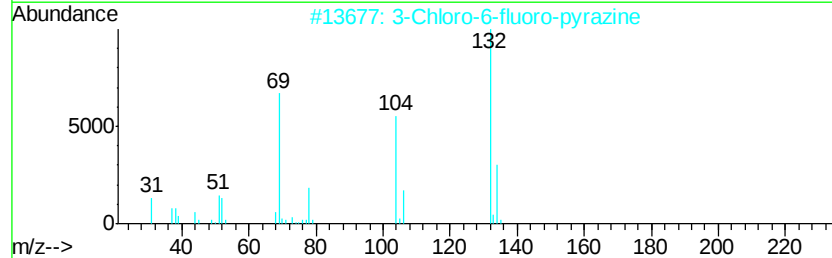
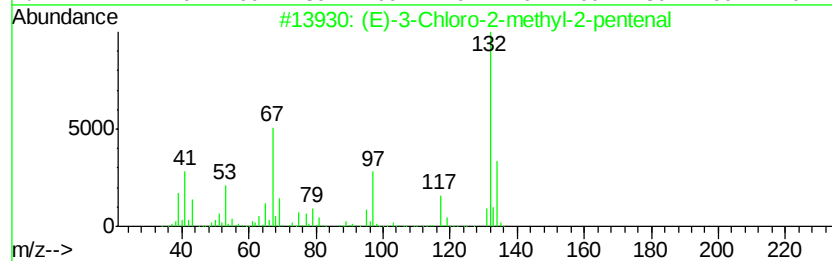
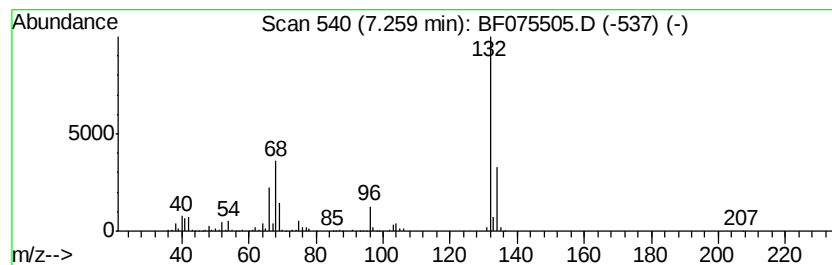
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 8 unknown7.26 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	55.61 ng	826565	1,4-Dichlorobenzene-d4	7.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.62	21.9	ng	326273	1	7.56	297259	20.0
3-Penten-2-one, 4...	4.57	15.4	ng	228530	1	7.56	297259	20.0
2-Pentanone, 4-hy...	5.35	124.8	ng	1855000	1	7.56	297259	20.0
Propane, 2-methox...	6.34	4.4	ng	65426	1	7.56	297259	20.0
unknown7.26	7.26	55.6	ng	826565	1	7.56	297259	20.0