

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
 Data File : BF075511.D
 Acq On : 14 Nov 2014 23:24
 Operator : TP / JJ
 Sample : PB80280BL
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB80280BL

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	44	47	50	rVB	415633	430290	24.93%	2.777%
2	1.761	56	59	63	rVB	41018	93114	5.39%	0.601%
3	1.830	63	65	70	rBV	66751	85880	4.98%	0.554%
4	1.967	75	77	83	rBV	245598	340698	19.74%	2.199%
5	4.584	304	306	312	rVB	26437	47006	2.72%	0.303%
6	5.339	370	372	379	rVB	531966	758264	43.93%	4.893%
7	5.841	413	416	418	rBV	1496924	1489617	86.30%	9.612%
8	6.344	458	460	463	rVB	27176	26099	1.51%	0.168%
9	7.087	523	525	528	rBV	1121428	1422462	82.41%	9.179%
10	7.259	537	540	542	rBV	1622667	1496755	86.71%	9.659%
11	7.545	563	565	568	rBV	241965	336216	19.48%	2.170%
12	7.739	580	582	584	rVB	1261237	1129803	65.45%	7.291%
13	8.242	623	626	628	rBV	994913	909943	52.71%	5.872%
14	9.133	701	704	706	rVB	474833	469111	27.18%	3.027%
15	10.471	819	821	824	rBV	1207101	1632306	94.56%	10.533%
16	11.305	892	894	897	rVB	363407	485489	28.13%	3.133%
17	12.288	978	980	983	rBV	914554	951264	55.11%	6.139%
18	13.156	1054	1056	1059	rBV	495583	481581	27.90%	3.108%
19	14.962	1212	1214	1217	rVB	36522	34090	1.97%	0.220%
20	15.157	1228	1231	1233	rBV	1619163	1726173	100.00%	11.139%
21	15.854	1290	1292	1294	rBV	21884	27598	1.60%	0.178%
22	16.448	1342	1344	1347	rBV	375917	524830	30.40%	3.387%
23	18.220	1496	1499	1502	rBV	378868	531708	30.80%	3.431%
24	18.334	1506	1509	1516	rVB2	14671	25800	1.49%	0.166%
25	19.351	1595	1598	1604	rVB2	11116	23257	1.35%	0.150%
26	20.734	1716	1719	1724	rBV6	6509	17329	1.00%	0.112%

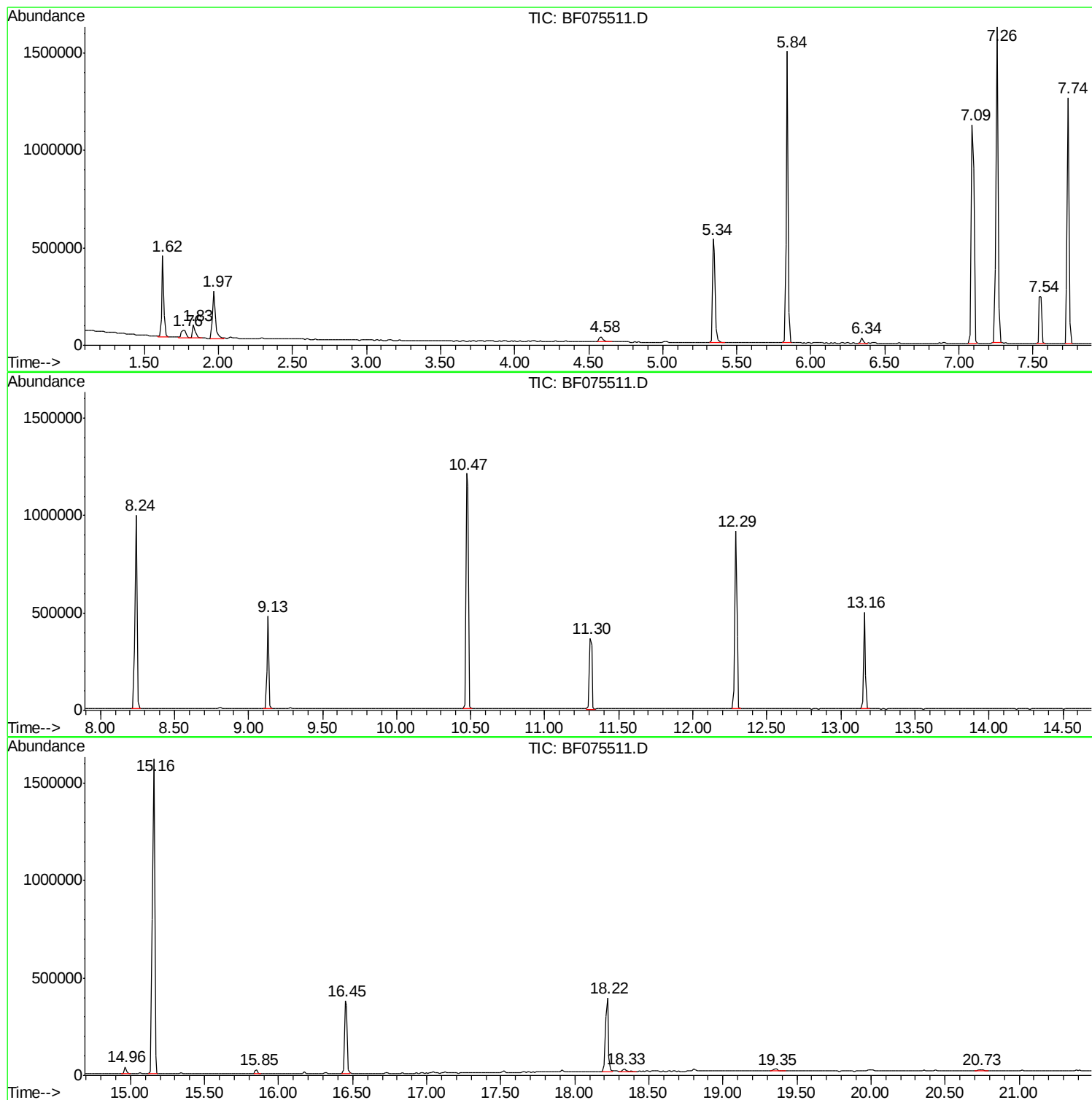
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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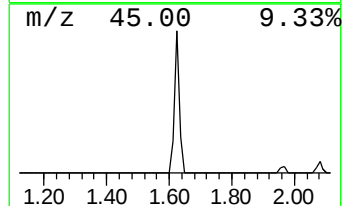
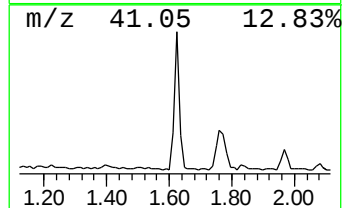
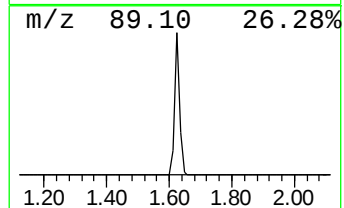
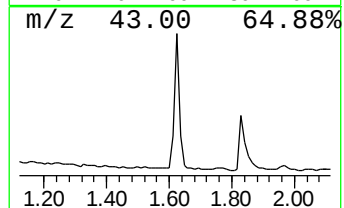
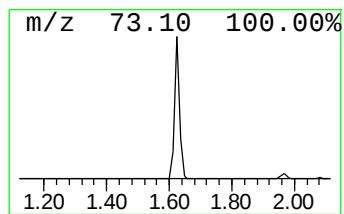
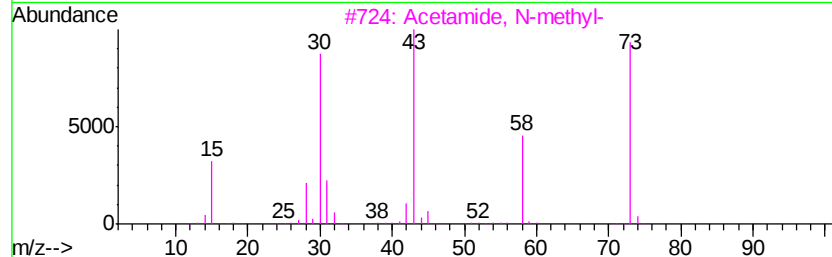
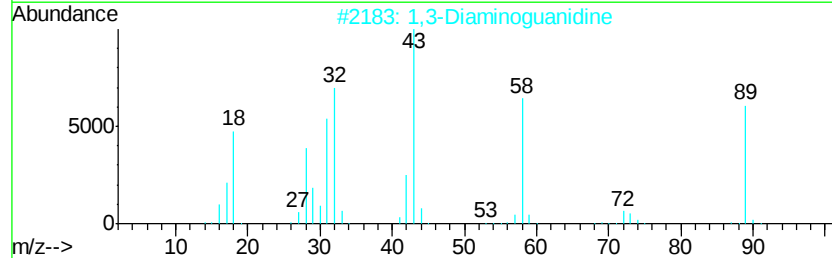
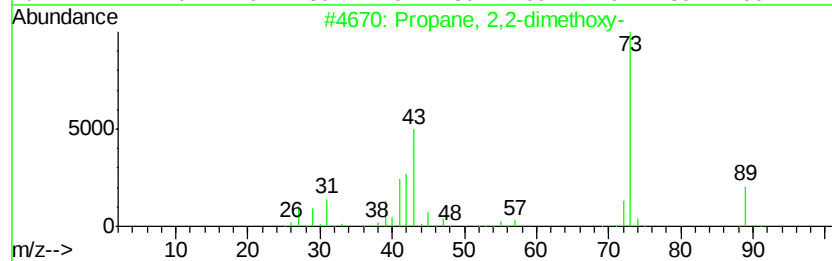
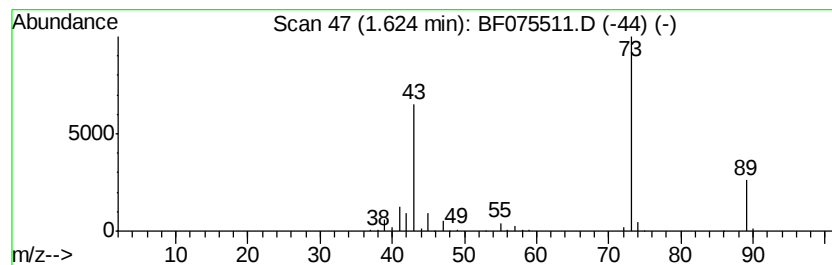
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	25.60 ng	430290	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	59
2			1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
3			Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
4			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	9



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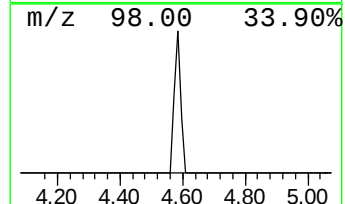
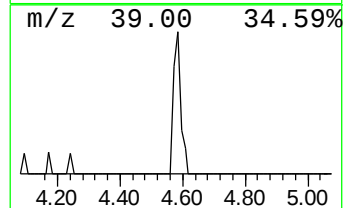
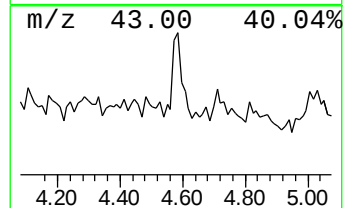
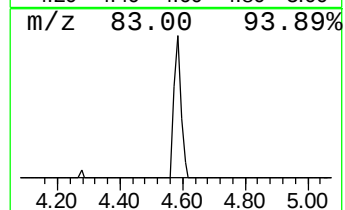
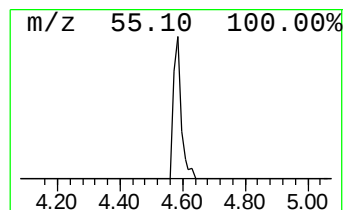
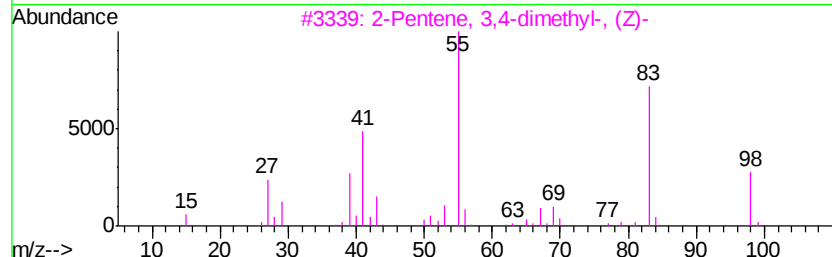
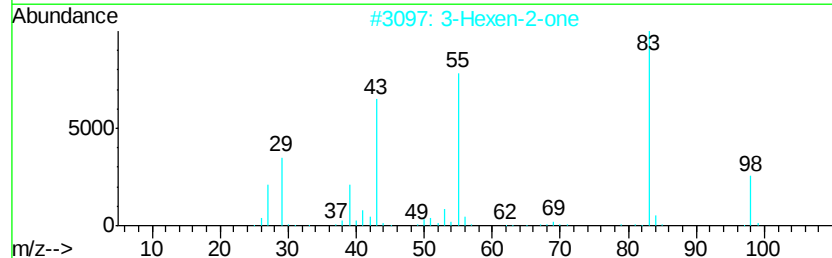
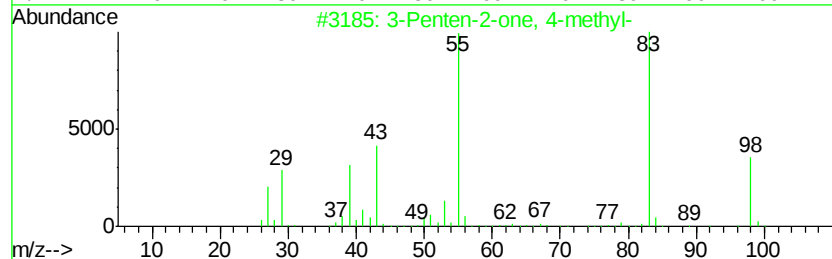
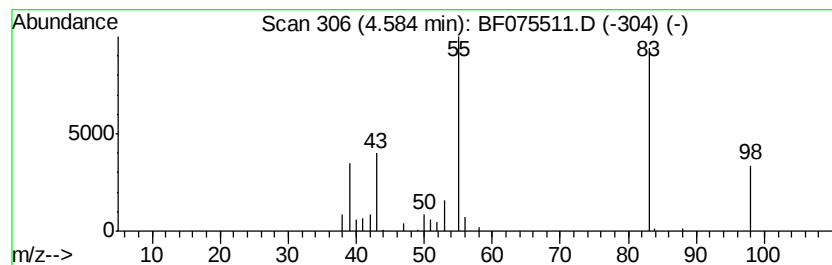
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	2.80 ng	47006	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	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	86
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
4		2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72
5		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72



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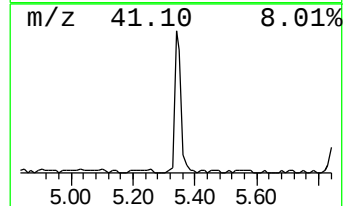
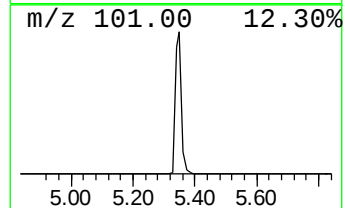
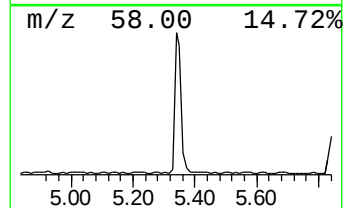
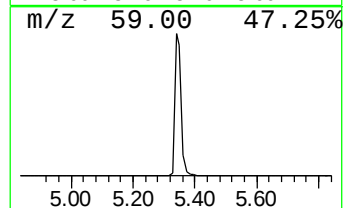
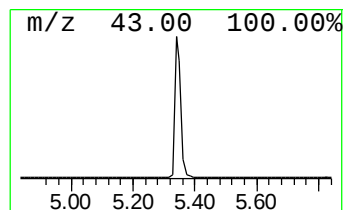
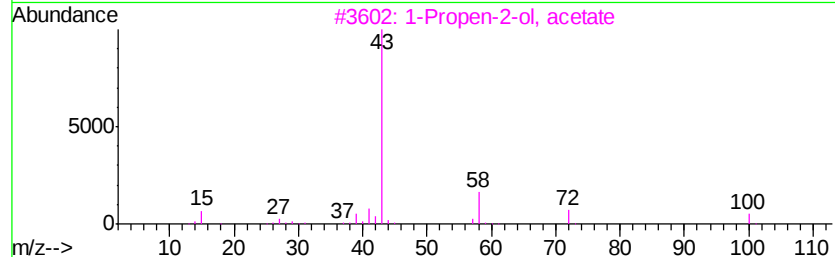
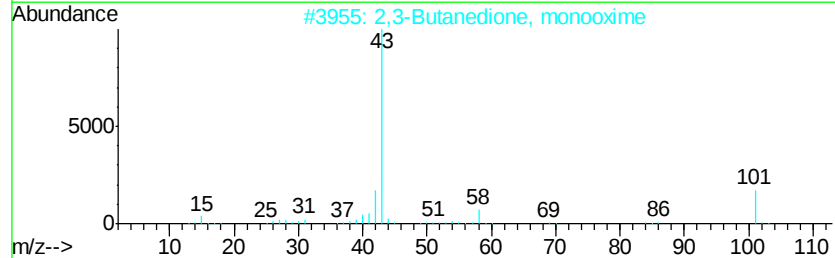
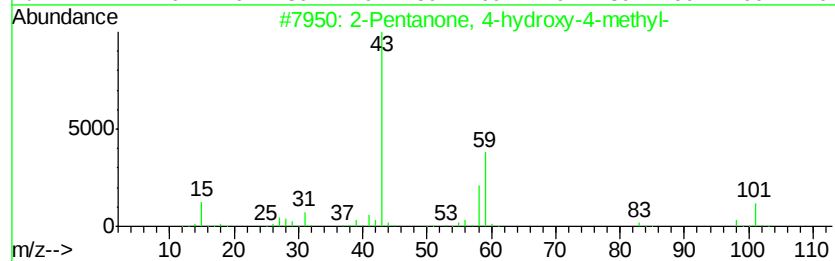
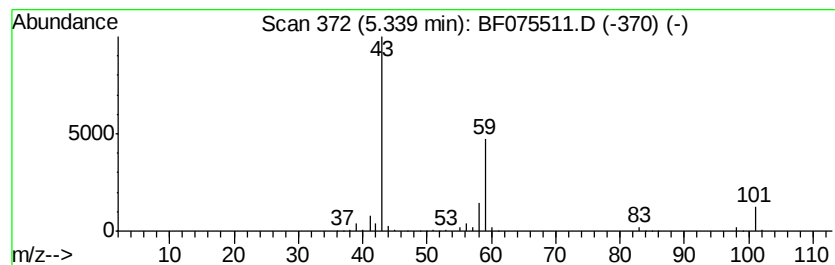
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	45.11 ng	758264	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		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4		2-Pentanone, 5-(acetyloxy)-	144	C7H12O3	005185-97-7	9
5		Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7



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Instrument :
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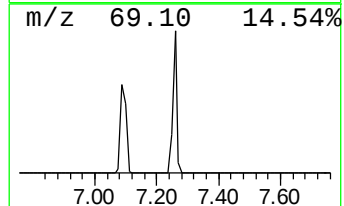
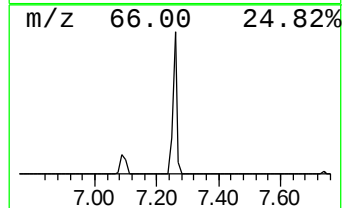
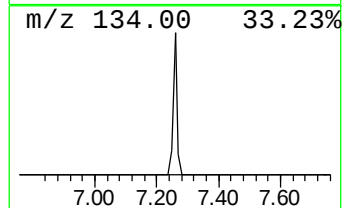
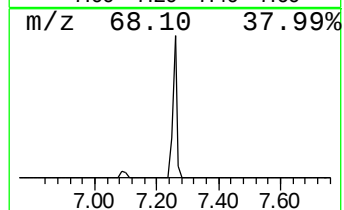
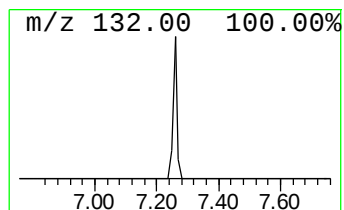
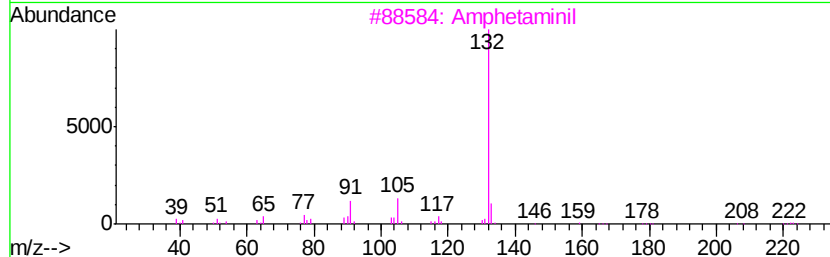
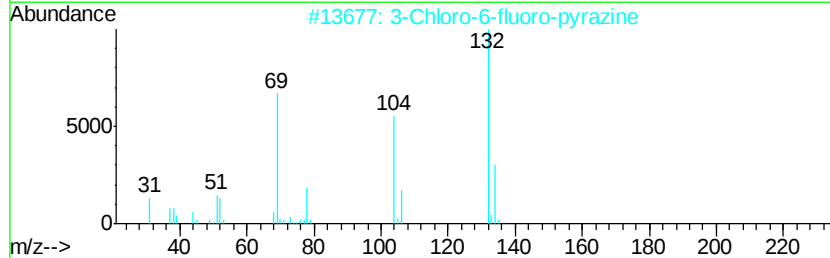
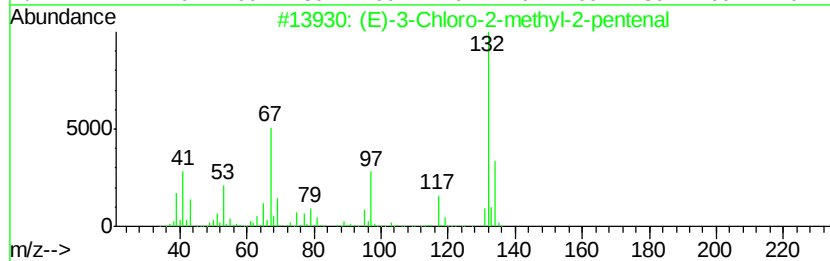
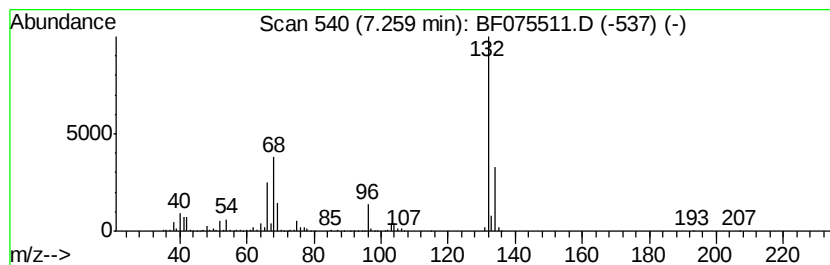
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 unknown7.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	89.04 ng	1496760	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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Aminoindole	132	C8H8N2	005192-03-0	12



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.62	25.6	ng	430290	1	7.56	336216	20.0
3-Penten-2-one, 4...	4.58	2.8	ng	47006	1	7.56	336216	20.0
2-Pentanone, 4-hy...	5.34	45.1	ng	758264	1	7.56	336216	20.0
unknown7.26	7.26	89.0	ng	1496760	1	7.56	336216	20.0