

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF041015\
 Data File : BF078411.D
 Acq On : 10 Apr 2015 20:51
 Operator : TP/IZ
 Sample : G1791-05
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 LS-SD09A

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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	1.012	9	11	14	rVB	271235	242900	31.11%	3.447%
2	1.127	18	21	23	rVB	75401	91392	11.71%	1.297%
3	1.264	31	33	38	rVB	56060	63512	8.14%	0.901%
4	1.527	55	56	63	rVB	8208	12677	1.62%	0.180%
5	1.618	63	64	76	rBV	193893	315359	40.39%	4.475%
6	4.521	316	318	325	rBV	44728	65801	8.43%	0.934%
7	5.116	367	370	376	rBV	413228	552483	70.77%	7.840%
8	6.453	485	487	495	rVB	607037	579977	74.29%	8.230%
9	6.567	495	497	500	rBV	621294	603043	77.24%	8.557%
10	6.853	520	522	525	rBV	156199	169941	21.77%	2.411%
11	7.036	536	538	541	rBV	305618	408602	52.34%	5.798%
12	7.562	581	584	586	rBV	318506	346287	44.36%	4.914%
13	8.430	658	660	663	rBV	188734	235751	30.20%	3.345%
14	9.150	722	723	725	rBV	9657	9418	1.21%	0.134%
15	9.779	776	778	781	rBV	695512	606854	77.73%	8.611%
16	10.293	821	823	825	rVB	40705	33615	4.31%	0.477%
17	10.590	847	849	852	rVB	325626	300171	38.45%	4.259%
18	11.493	926	928	932	rBV	20308	19046	2.44%	0.270%
19	11.562	932	934	937	rBV	456225	467081	59.83%	6.628%
20	12.419	1006	1009	1011	rBV	250029	318393	40.78%	4.518%
21	14.408	1180	1183	1185	rBV	788999	780700	100.00%	11.078%
22	15.597	1284	1287	1291	rBV	14658	26964	3.45%	0.383%
23	15.677	1291	1294	1297	rVB	380067	393180	50.36%	5.579%
24	17.197	1424	1427	1430	rBV3	3922	9604	1.23%	0.136%
25	17.403	1442	1445	1448	rBV	292372	385870	49.43%	5.476%
26	17.585	1457	1461	1463	rVB4	4917	8574	1.10%	0.122%

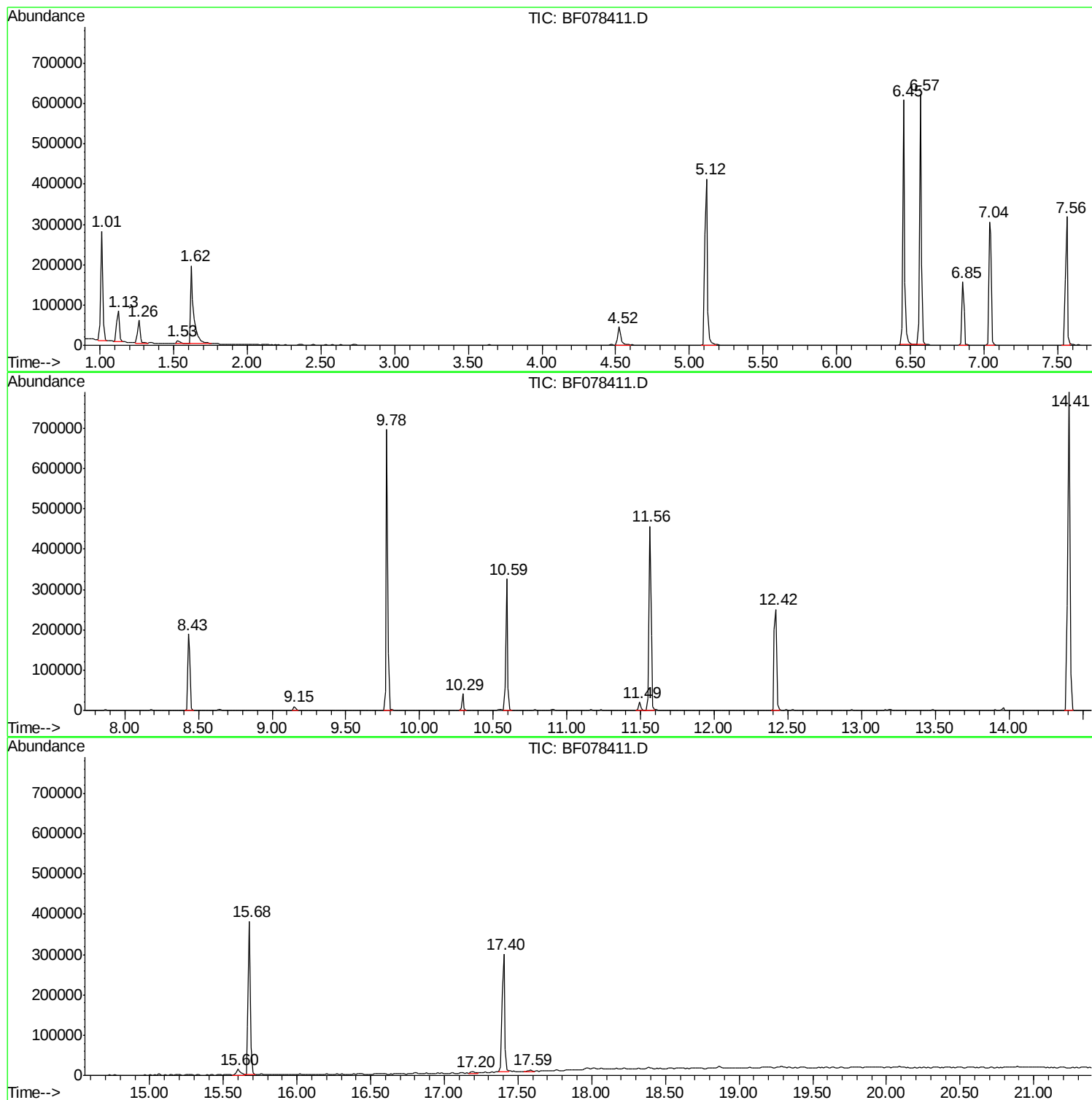
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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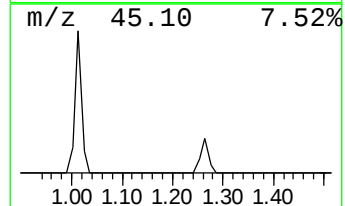
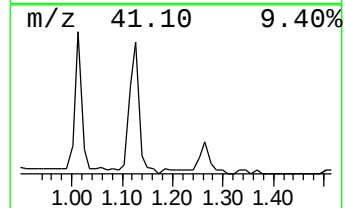
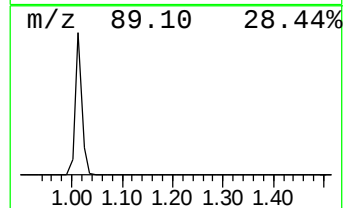
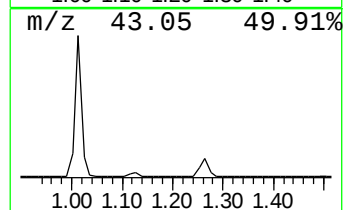
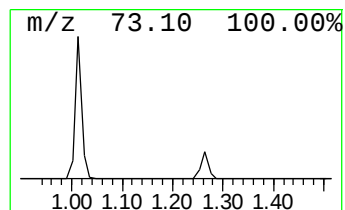
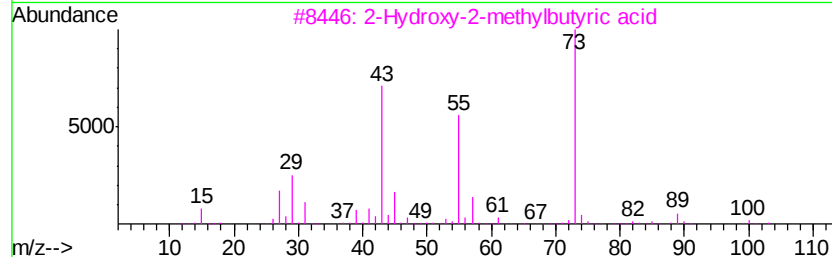
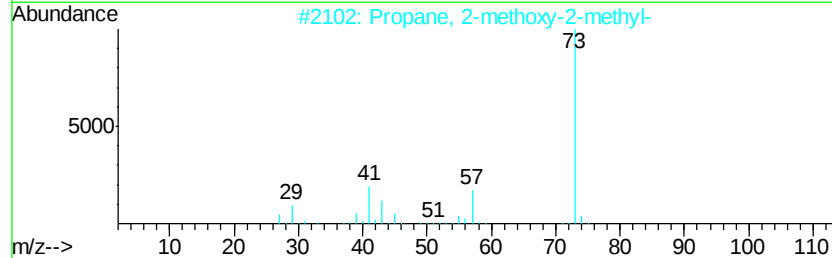
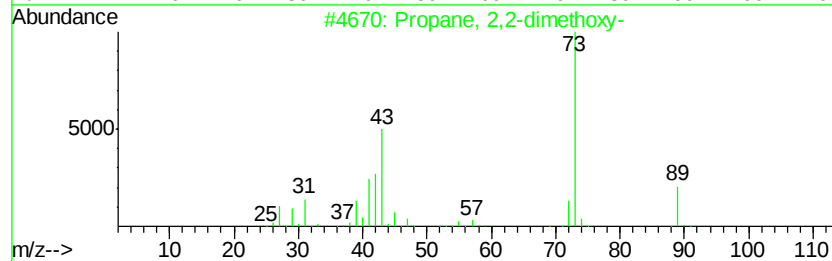
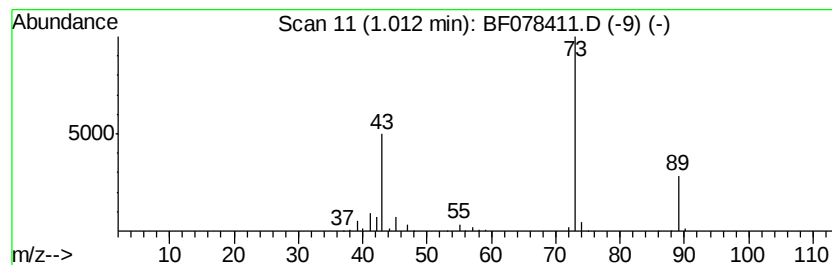
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
1.01	28.59 ng	242900	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	9



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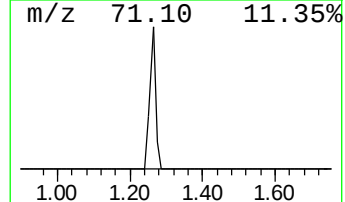
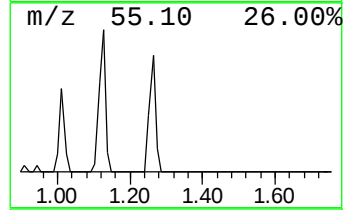
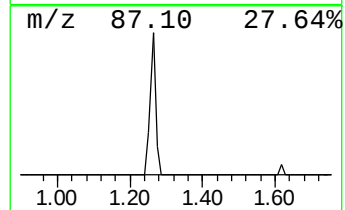
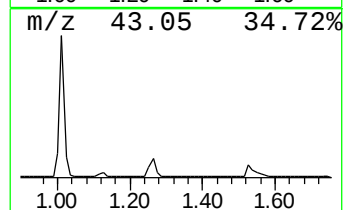
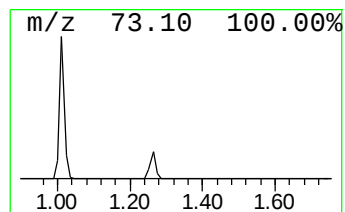
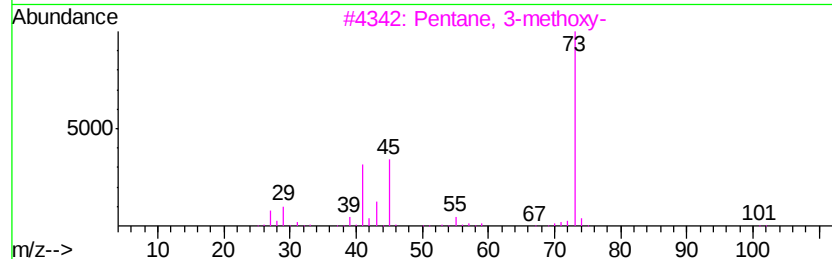
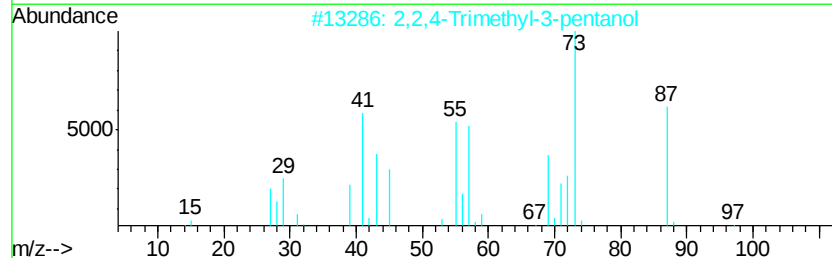
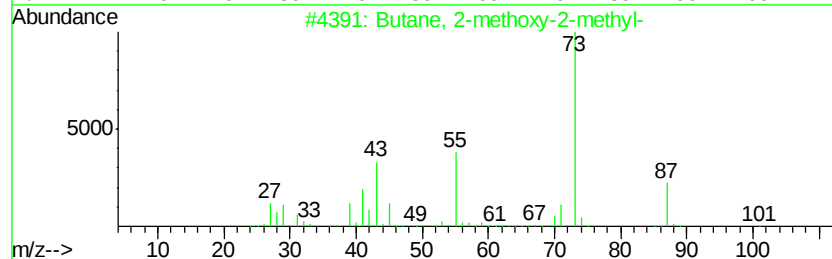
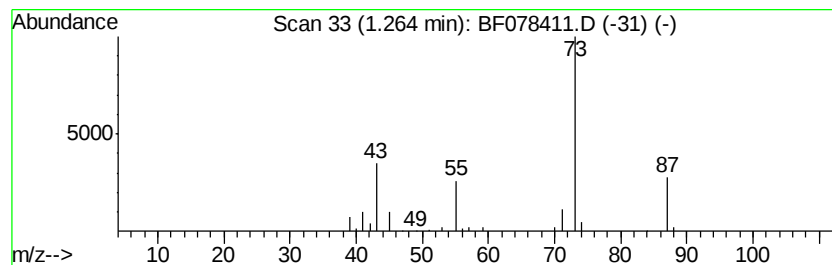
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	7.47 ng	63512	1,4-Dichlorobenzene-d4	6.85

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	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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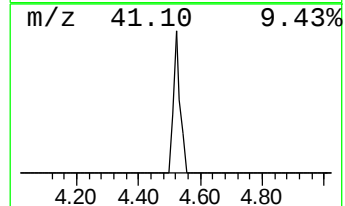
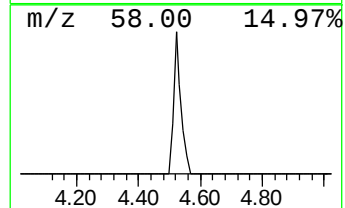
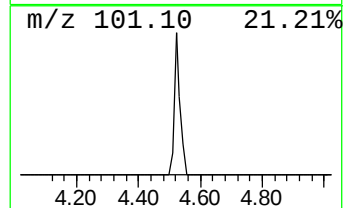
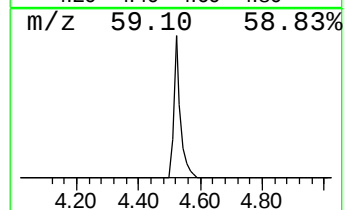
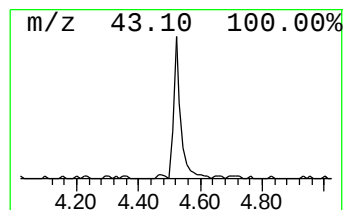
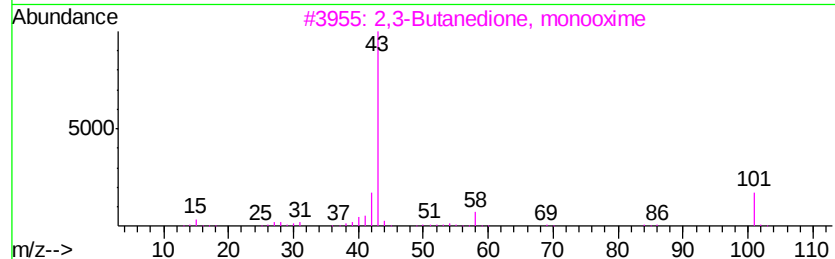
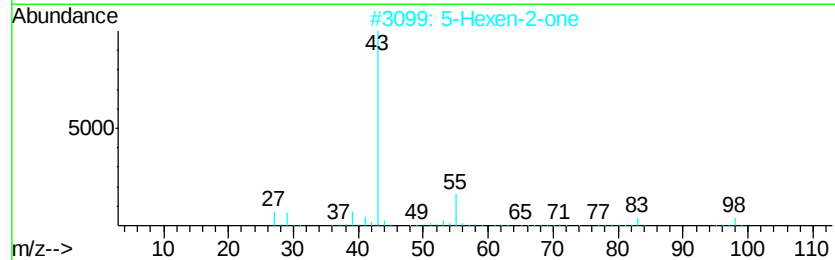
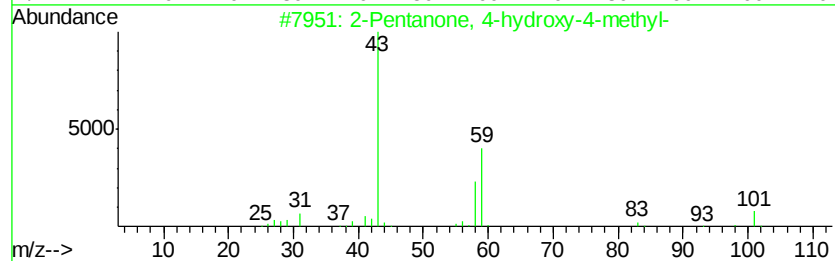
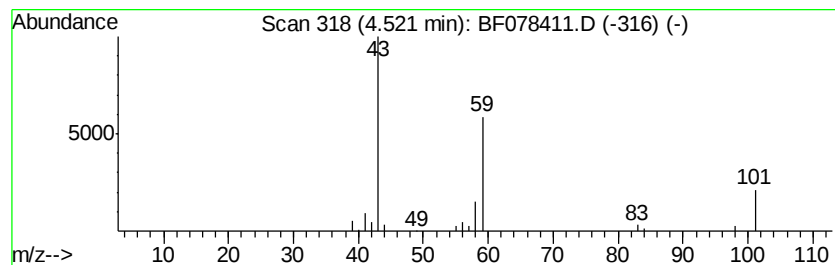
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	7.74 ng	65801	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42		
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
4	3-Octanol	130	C8H18O	000589-98-0	9		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9		



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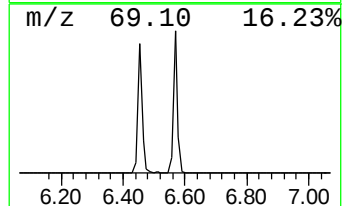
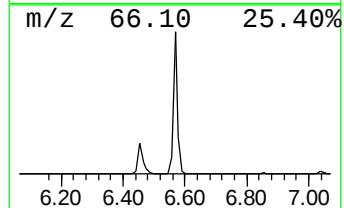
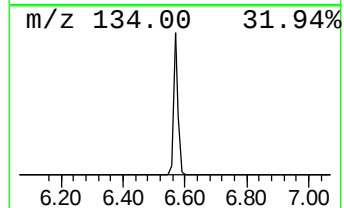
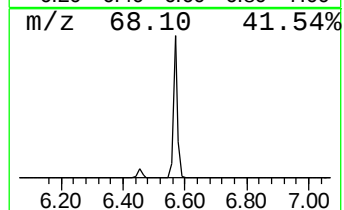
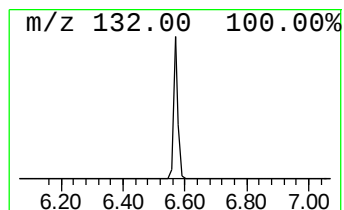
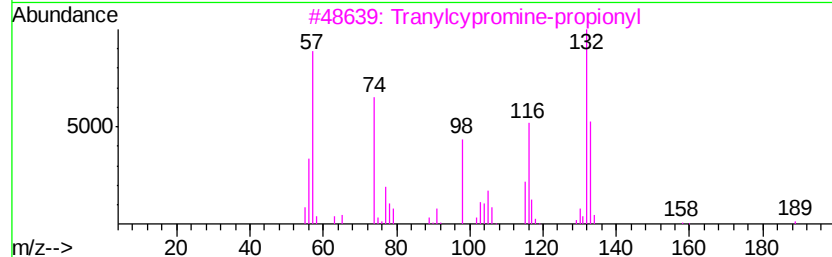
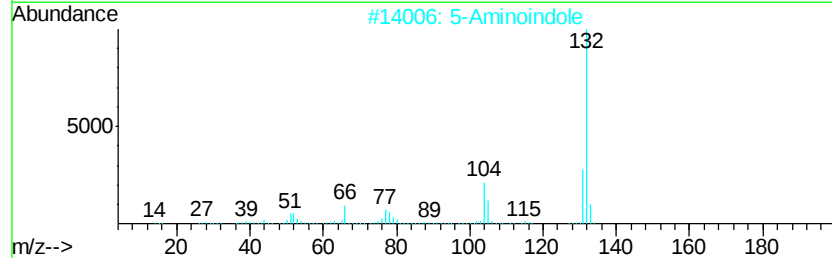
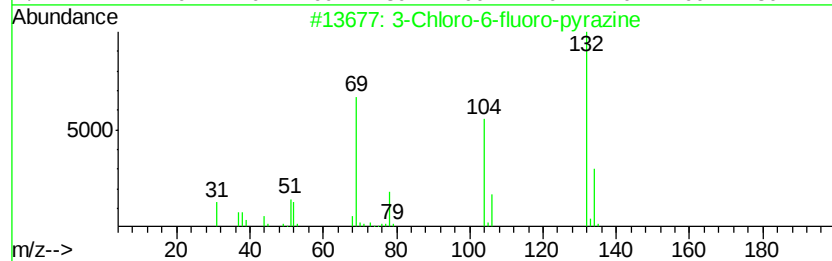
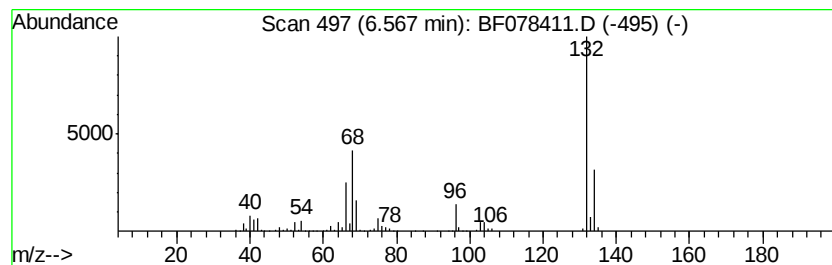
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	70.97 ng	603043	1,4-Dichlorobenzene-d4	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	1.01	28.6	ng	242900	1	6.85	169941	20.0
Butane, 2-methoxy...	1.26	7.5	ng	63512	1	6.85	169941	20.0
2-Pentanone, 4-hy...	4.52	7.7	ng	65801	1	6.85	169941	20.0
unknown6.57	6.57	71.0	ng	603043	1	6.85	169941	20.0