

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012016\
 Data File : BF084572.D
 Acq On : 20 Jan 2016 18:45
 Operator : SJ/UM
 Sample : H1159-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SULFURCAKE

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-BF123115.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	2.407	21	28	32	rVB2	24193	88116	1.12%	0.135%
2	2.567	39	42	46	rVB	193575	279612	3.56%	0.428%
3	4.293	191	193	199	rVB	247591	392334	5.00%	0.601%
4	4.979	249	253	267	rVB	3203485	4992928	63.58%	7.643%
5	5.402	287	290	292	rBV	4328684	5985683	76.22%	9.163%
6	5.790	322	324	327	rVB	342290	303765	3.87%	0.465%
7	6.430	377	380	382	rBV	5276479	5493894	69.96%	8.410%
8	6.556	388	391	393	rBV	6008739	6543027	83.32%	10.016%
9	6.773	408	410	413	rBV	990538	1345677	17.14%	2.060%
10	6.933	422	424	427	rVB	4461110	4610048	58.70%	7.057%
11	7.345	457	460	463	rBV	3583862	3823310	48.68%	5.853%
12	8.065	520	523	527	rBV2	2246505	2635232	33.56%	4.034%
13	8.773	583	585	587	rVV	252853	224093	2.85%	0.343%
14	8.876	591	594	596	rVB	140499	126414	1.61%	0.194%
15	9.150	614	618	620	rBV	6973239	7853286	100.00%	12.022%
16	9.825	674	677	678	rBV	1853213	2131348	27.14%	3.263%
17	9.848	678	679	681	rVB	268771	271907	3.46%	0.416%
18	10.019	692	694	697	rBV	127066	159457	2.03%	0.244%
19	10.362	723	724	727	rVB	136671	156834	2.00%	0.240%
20	10.613	743	746	748	rBV	4663295	4897432	62.36%	7.497%
21	11.299	804	806	810	rBV	1536880	2384740	30.37%	3.650%
22	12.899	943	946	949	rBV	6825085	7202383	91.71%	11.025%
23	13.940	1035	1037	1040	rBV	1997928	1971058	25.10%	3.017%
24	15.357	1157	1161	1163	rBV	958358	1454217	18.52%	2.226%

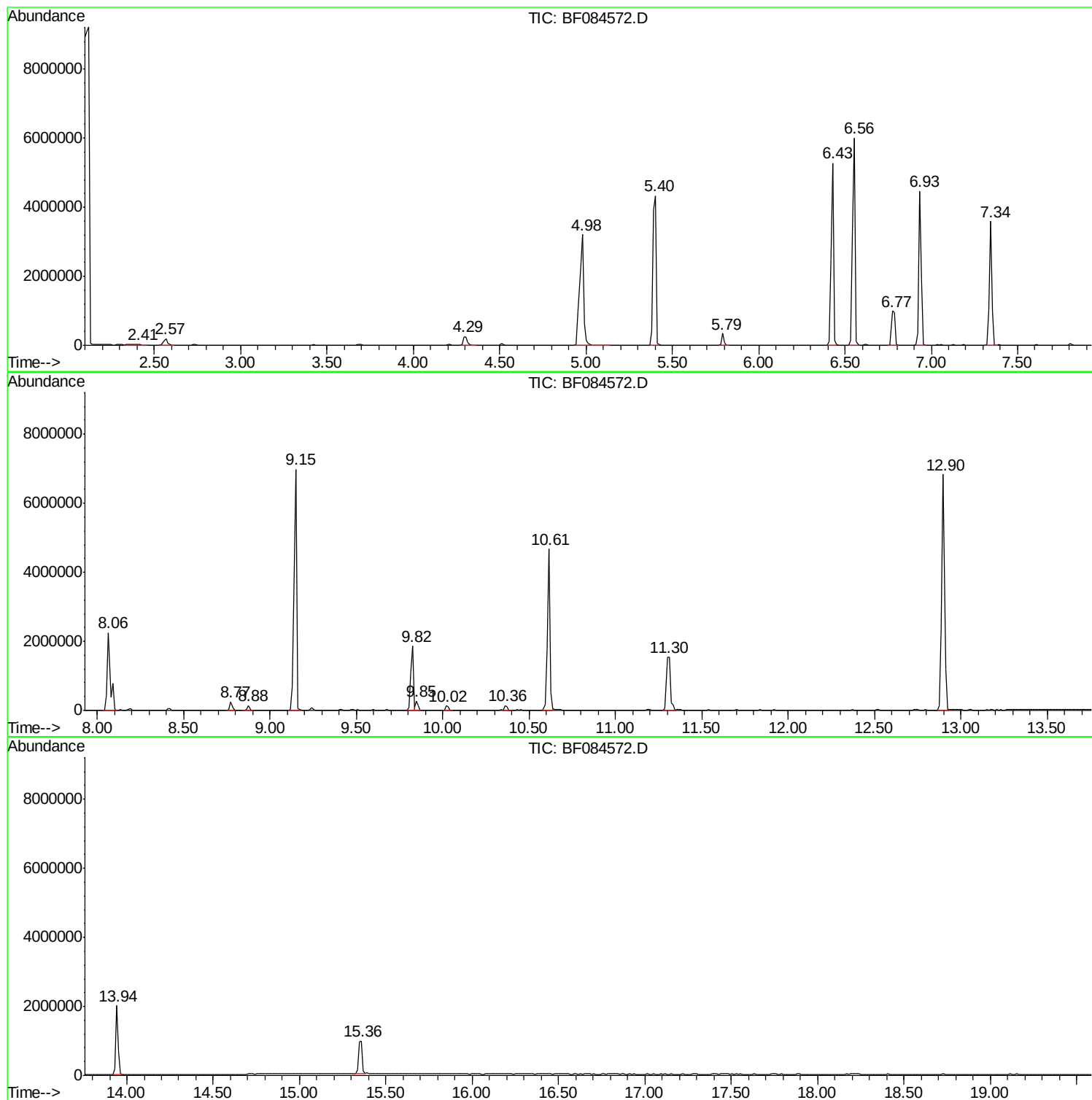
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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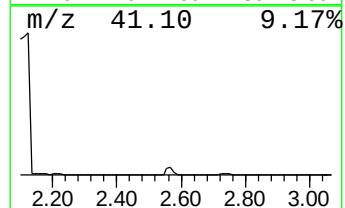
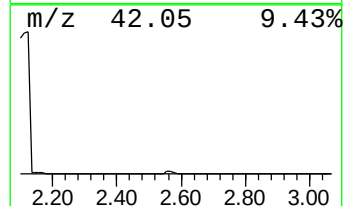
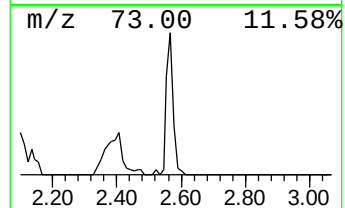
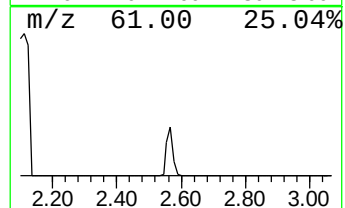
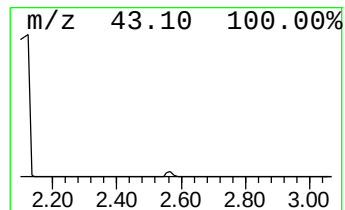
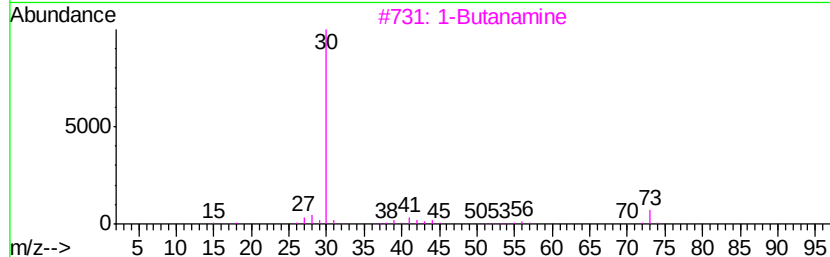
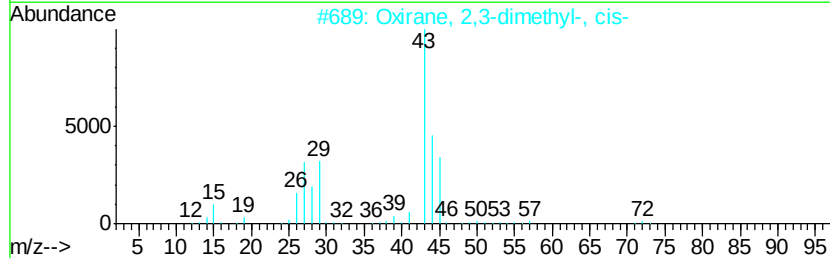
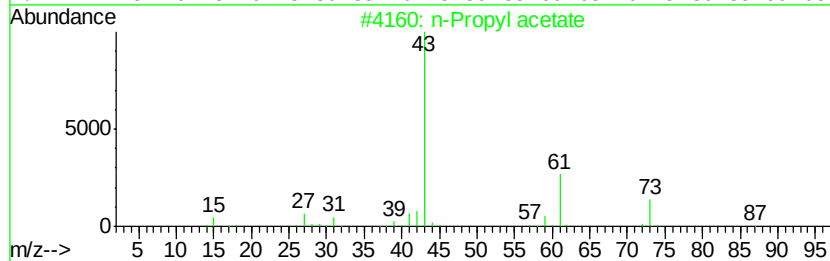
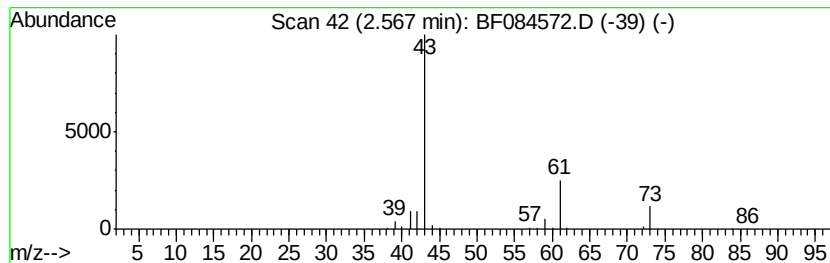
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.57	4.16 ng	279612	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
3		1-Butanamine	73	C4H11N	000109-73-9	5
4		Isobutylamine	73	C4H11N	000078-81-9	4
5		Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	4



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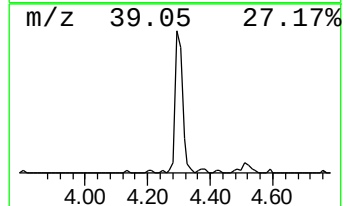
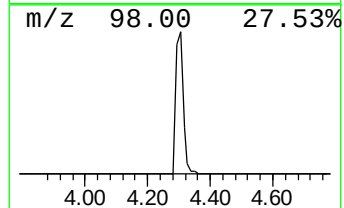
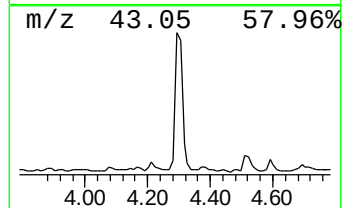
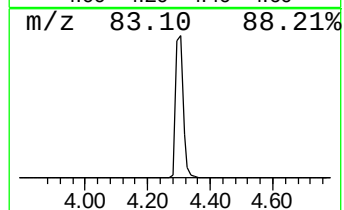
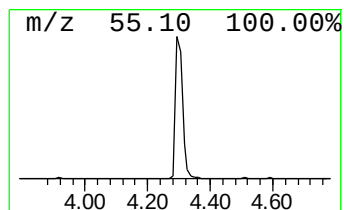
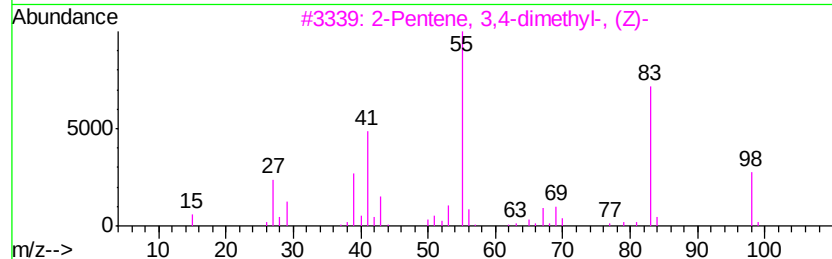
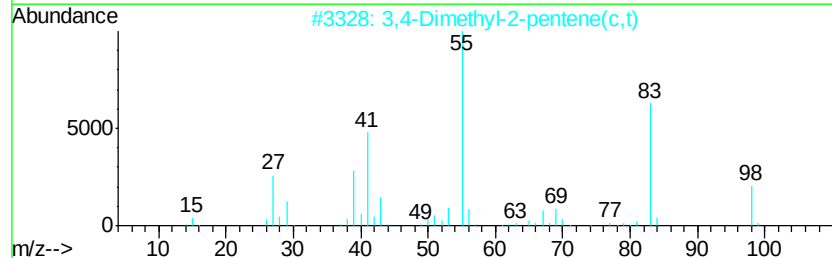
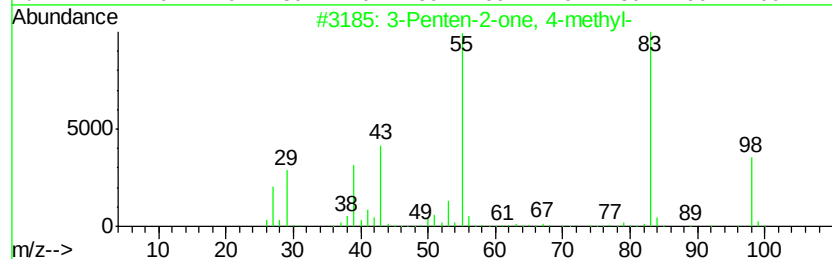
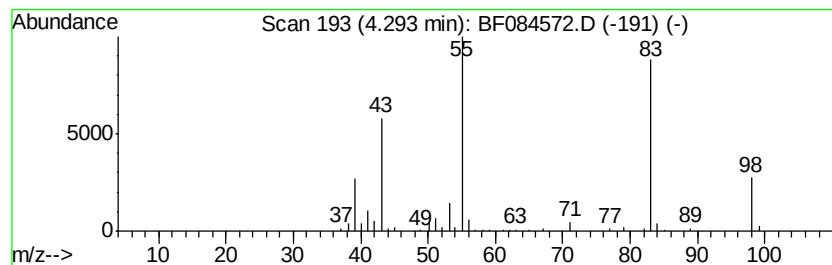
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.29	5.83 ng	392334	1,4-Dichlorobenzene-d4	6.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
5			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	72



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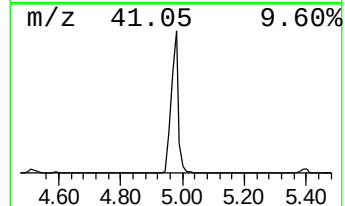
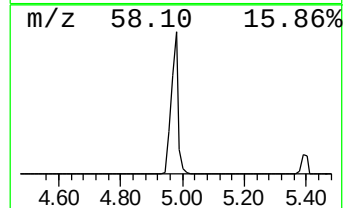
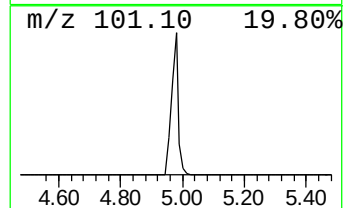
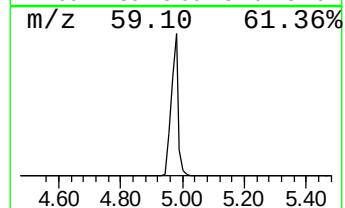
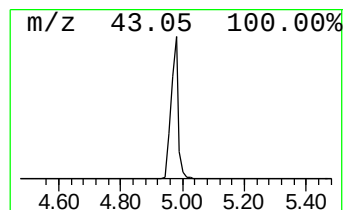
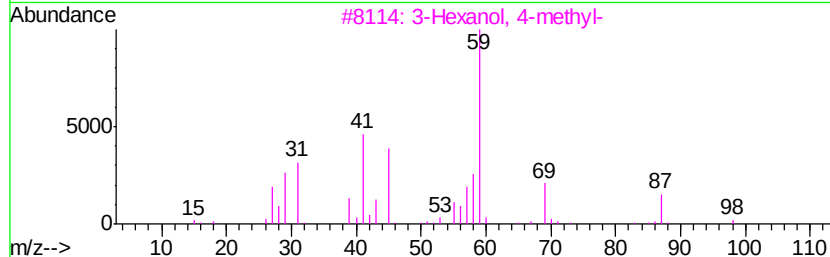
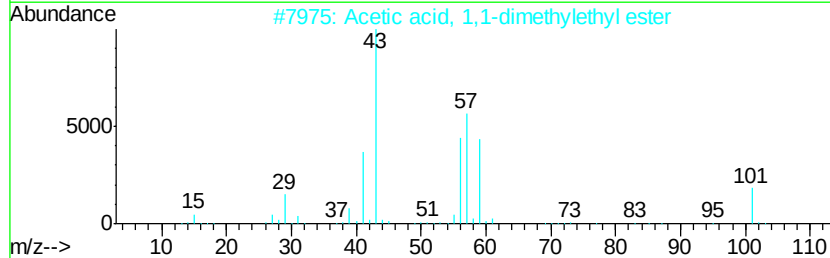
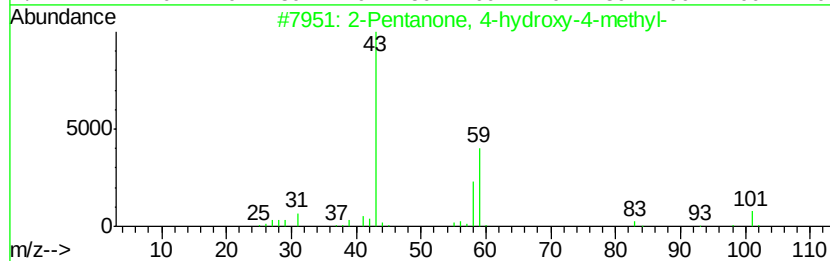
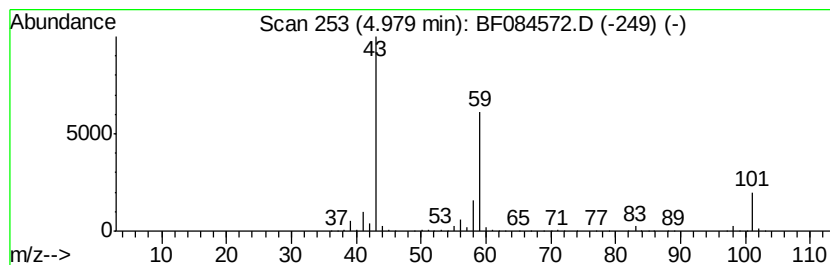
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	74.21 ng	4992930	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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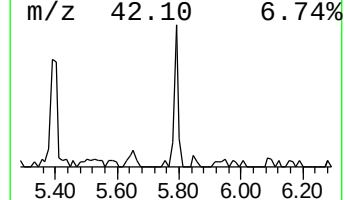
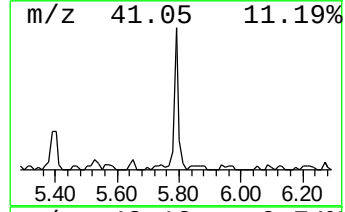
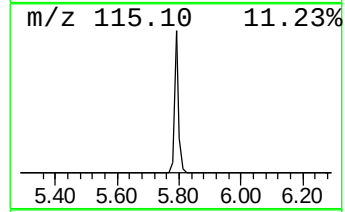
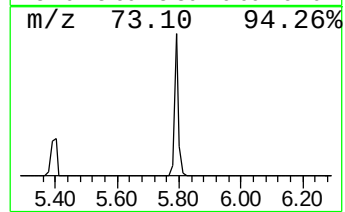
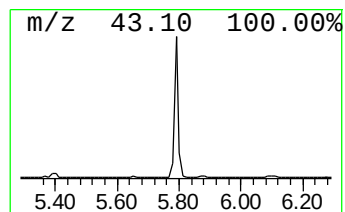
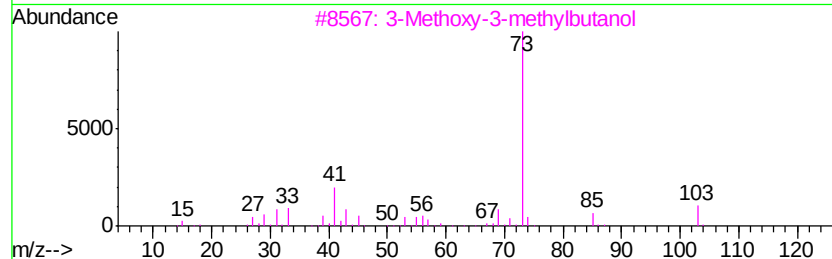
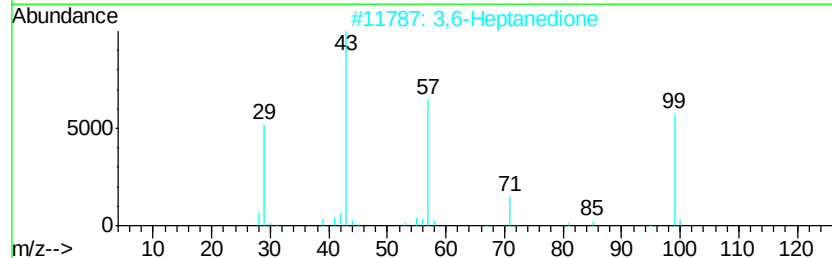
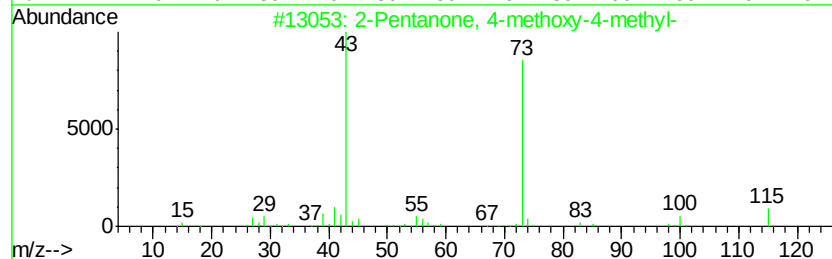
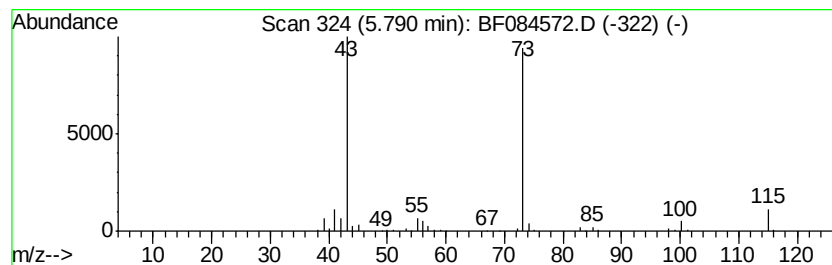
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.79	4.51 ng	303765	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		3,6-Heptanedione	128	C7H12O2	001703-51-1	23
3		3-Methoxy-3-methylbutanol	118	C6H14O2	056539-66-3	17
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	10
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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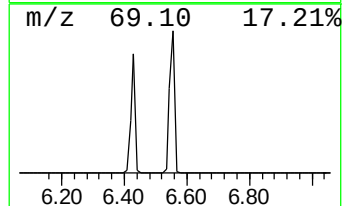
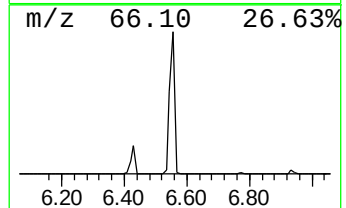
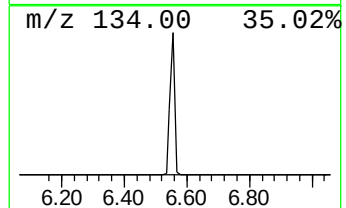
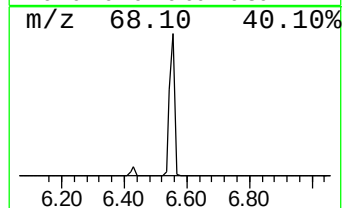
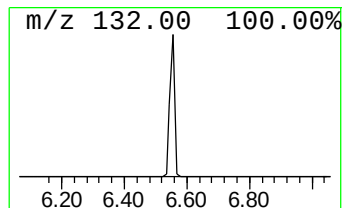
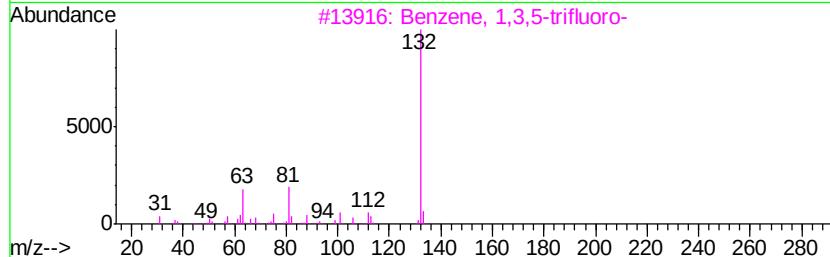
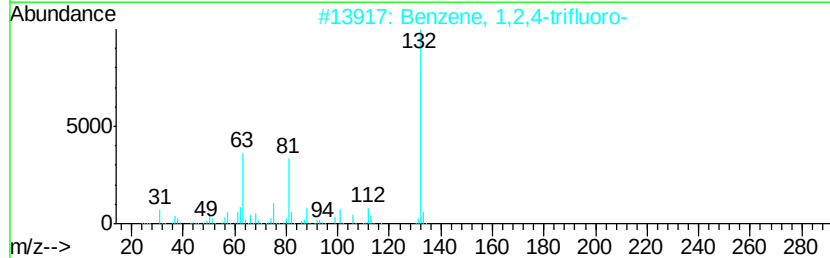
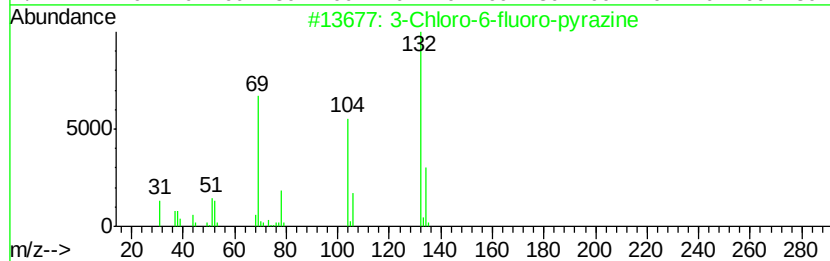
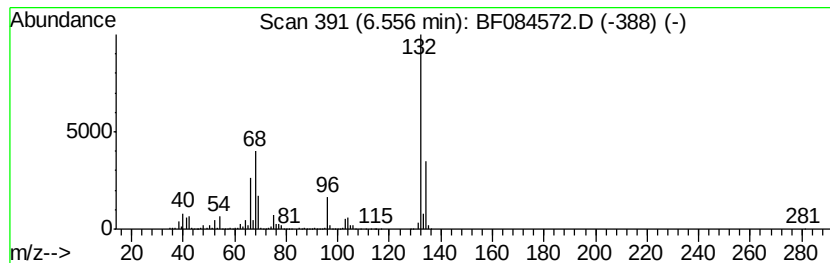
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Peak Number 5 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	97.25 ng	6543030	1,4-Dichlorobenzene-d4	6.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.57	4.2	ng	279612	1	6.78	1345680	20.0
3-Penten-2-one, 4...	4.29	5.8	ng	392334	1	6.78	1345680	20.0
2-Pentanone, 4-hy...	4.98	74.2	ng	4992930	1	6.78	1345680	20.0
2-Pentanone, 4-me...	5.79	4.5	ng	303765	1	6.78	1345680	20.0
unknown6.56	6.56	97.3	ng	6543030	1	6.78	1345680	20.0