

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031815\
 Data File : BF077820.D
 Acq On : 19 Mar 2015 4:44
 Operator : TP/IZ
 Sample : G1544-03
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-9(7-9)

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-BF031115.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	1.321	35	38	40	rBV	3780364	4450936	100.00%	33.278%
2	1.435	45	48	51	rBV	65548	108076	2.43%	0.808%
3	1.607	60	63	66	rVB	55201	64566	1.45%	0.483%
4	1.790	77	79	85	rBV	38115	54472	1.22%	0.407%
5	4.933	352	354	361	rBB	92217	121315	2.73%	0.907%
6	5.458	397	400	403	rBV	708227	728044	16.36%	5.443%
7	6.739	510	512	515	rBV	618053	698023	15.68%	5.219%
8	6.876	521	524	527	rBV	834545	762894	17.14%	5.704%
9	7.162	547	549	552	rBB	236477	210362	4.73%	1.573%
10	7.344	563	565	568	rBV	661554	622745	13.99%	4.656%
11	7.859	607	610	612	rBV	486832	476411	10.70%	3.562%
12	8.739	685	687	689	rBV	353379	310851	6.98%	2.324%
13	10.088	802	805	807	rBV	1025411	1040994	23.39%	7.783%
14	10.590	847	849	852	rBV	45210	49620	1.11%	0.371%
15	10.910	875	877	879	rBV	347363	348546	7.83%	2.606%
16	11.893	960	963	965	rBV	417747	602340	13.53%	4.504%
17	12.751	1035	1038	1040	rBV	354747	377010	8.47%	2.819%
18	14.739	1210	1212	1215	rBV	885149	1251815	28.12%	9.359%
19	15.928	1313	1316	1319	rBV	78068	108239	2.43%	0.809%
20	16.031	1323	1325	1328	rBV	345575	479125	10.76%	3.582%
21	17.791	1477	1479	1487	rBV	305342	508527	11.43%	3.802%

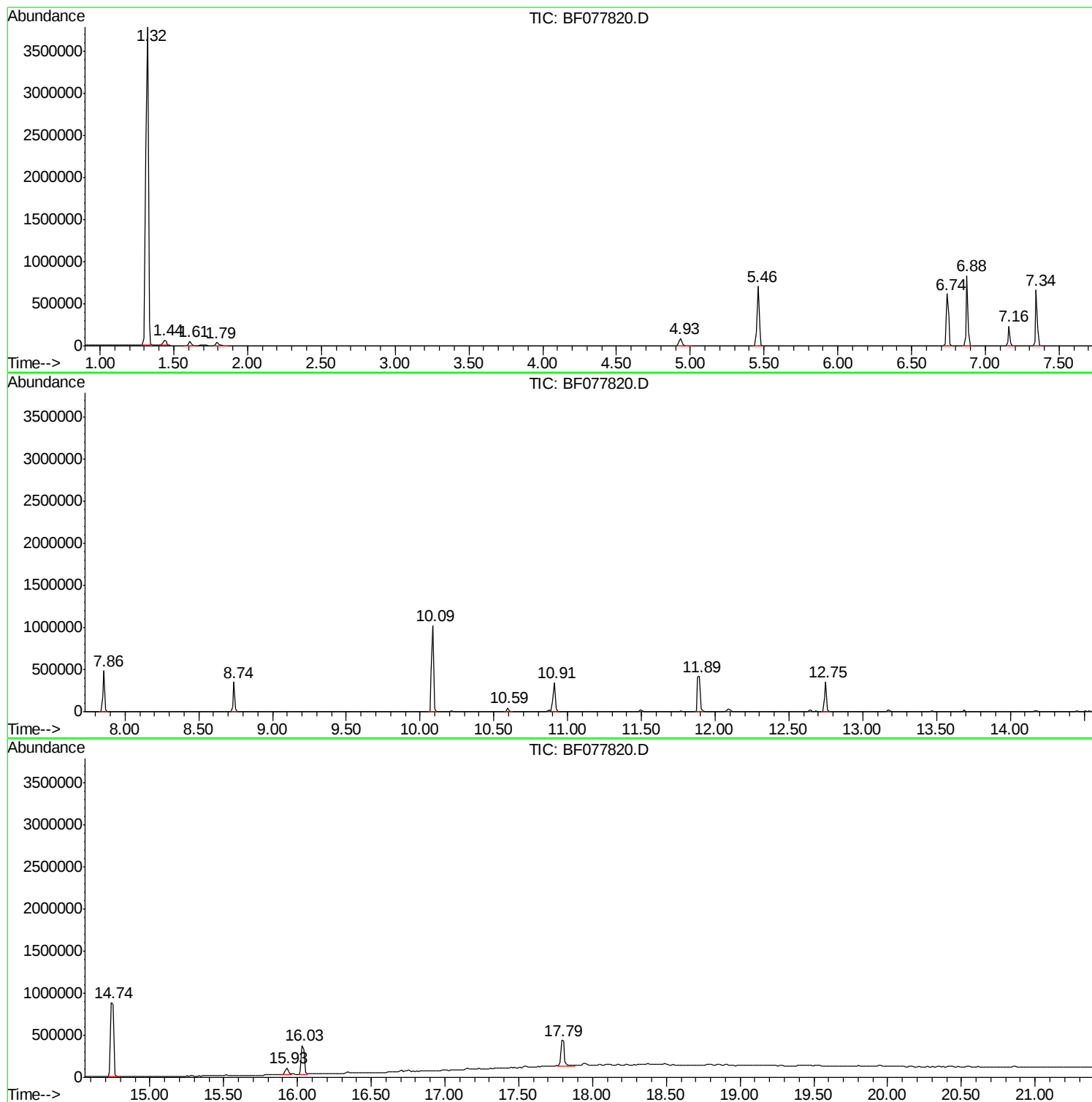
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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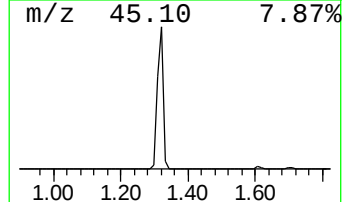
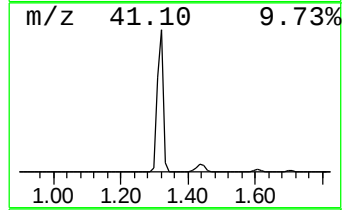
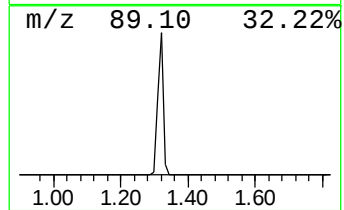
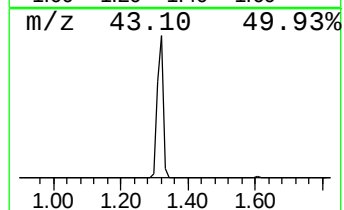
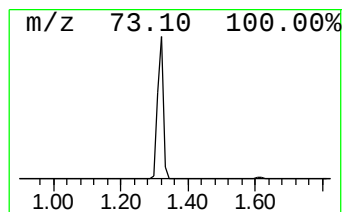
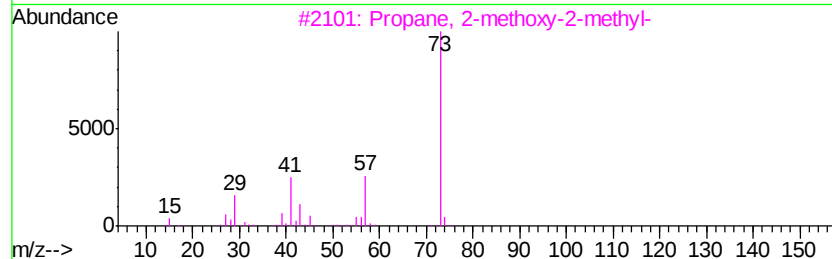
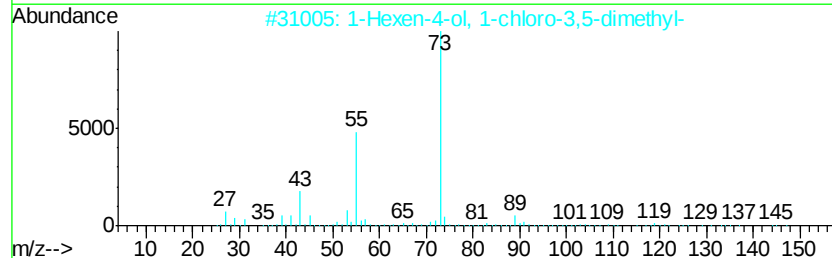
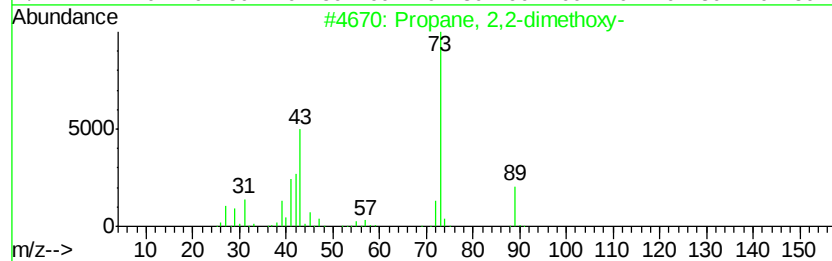
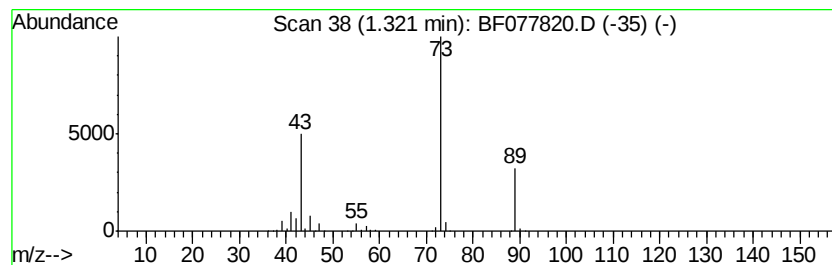
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	423.17 ng	4450940	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	5



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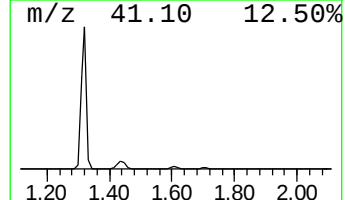
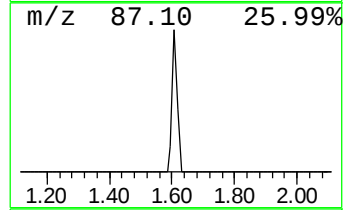
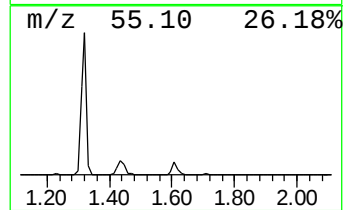
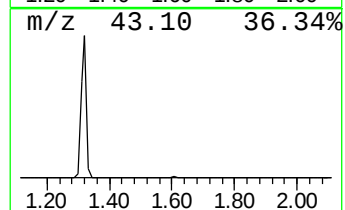
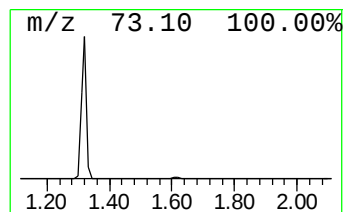
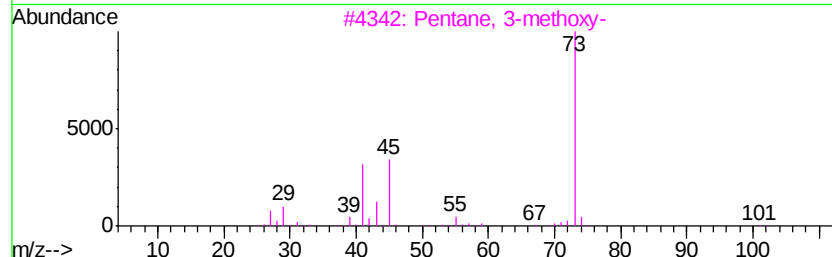
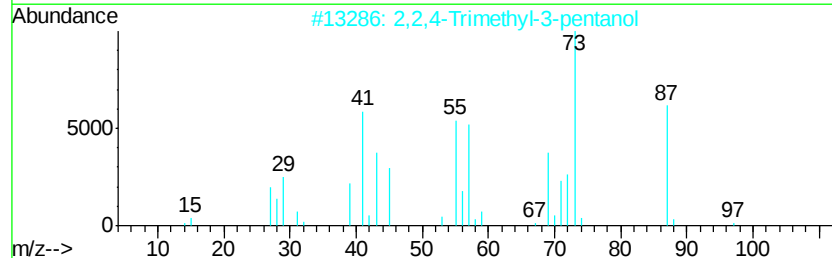
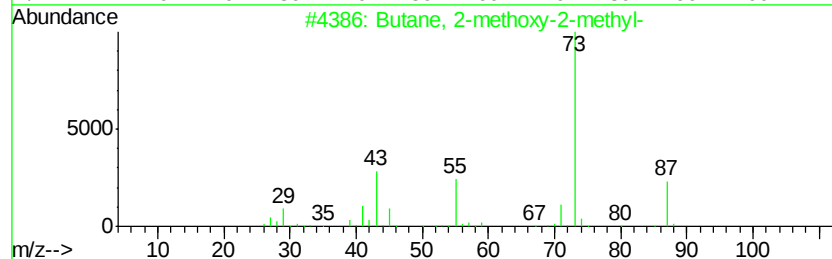
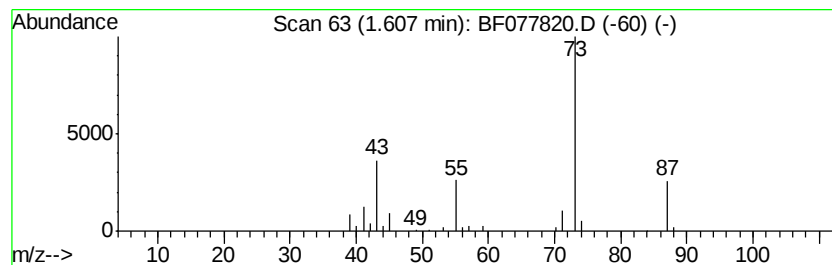
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Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.61	6.14 ng	64566	1,4-Dichlorobenzene-d4	7.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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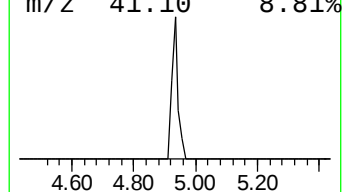
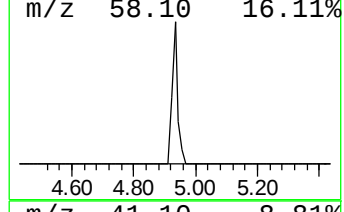
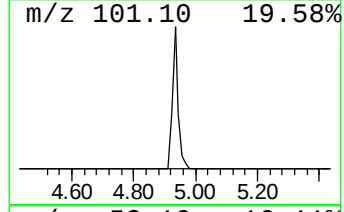
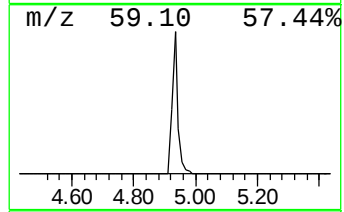
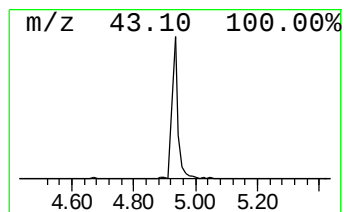
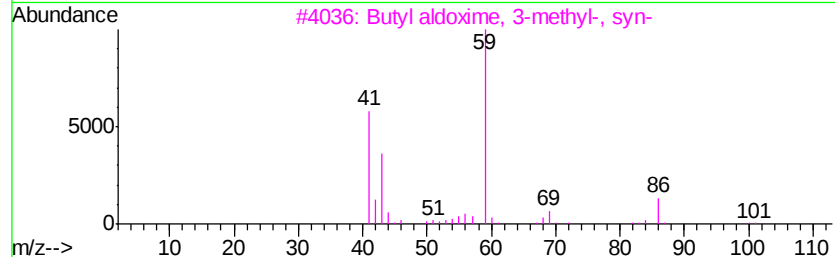
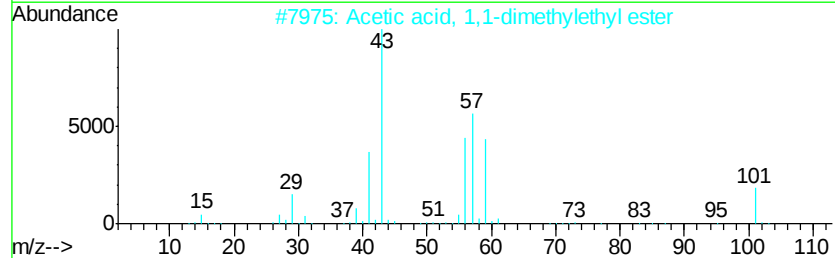
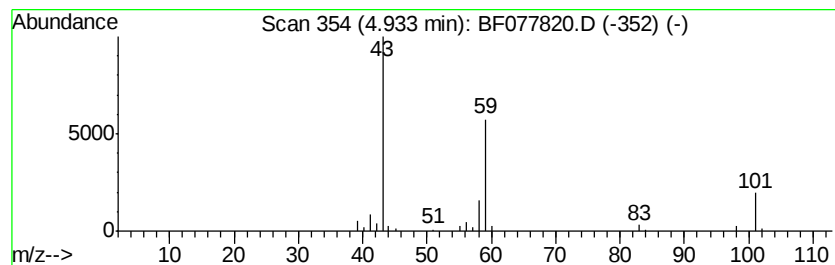
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Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	11.53 ng	121315	1,4-Dichlorobenzene-d4	7.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40	
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39	
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25	
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	23	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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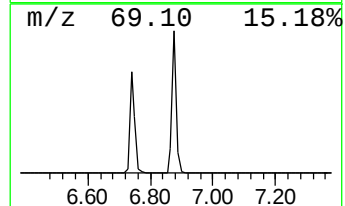
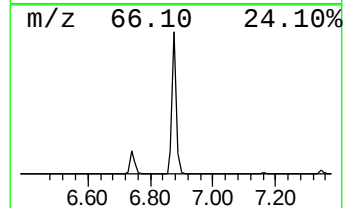
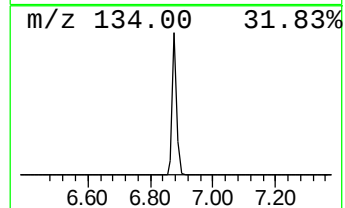
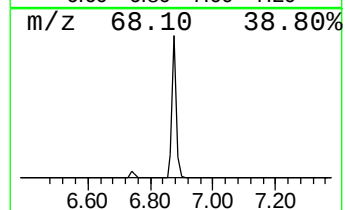
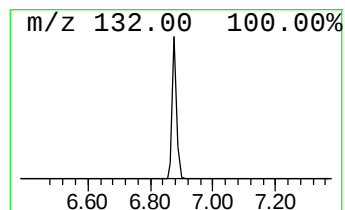
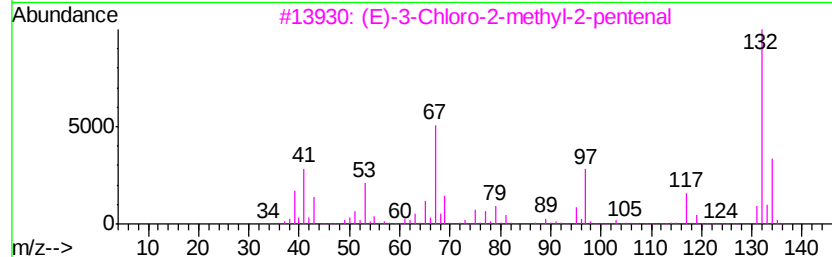
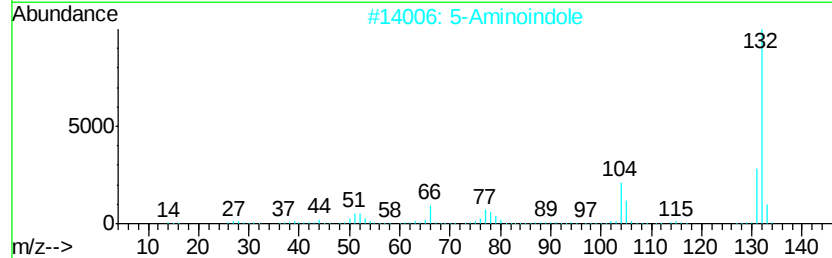
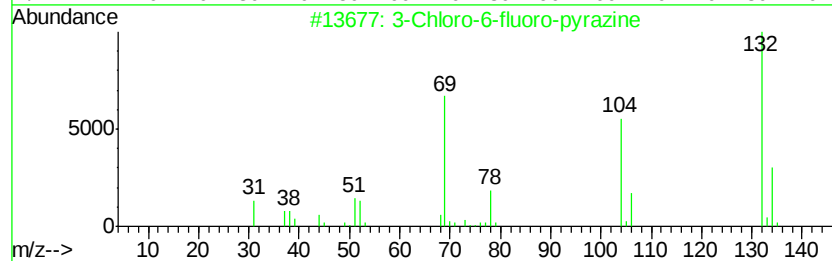
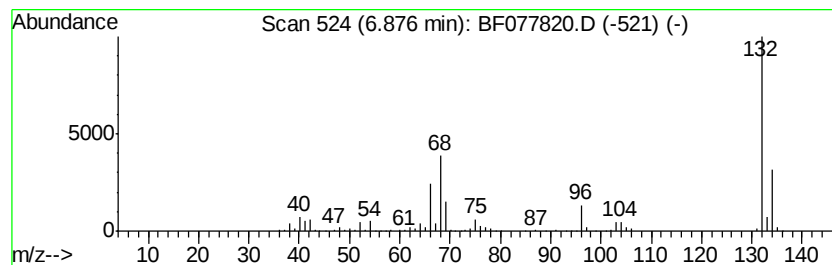
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 unknown6.88 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.88	72.53 ng	762894	1,4-Dichlorobenzene-d4	7.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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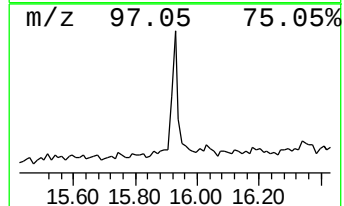
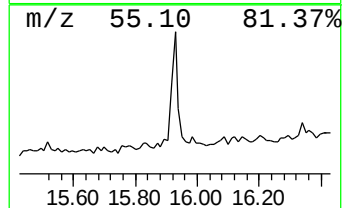
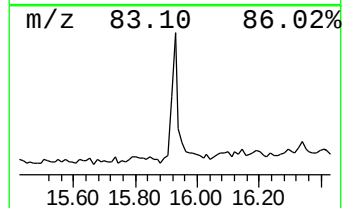
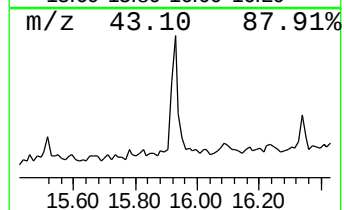
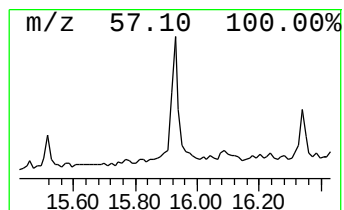
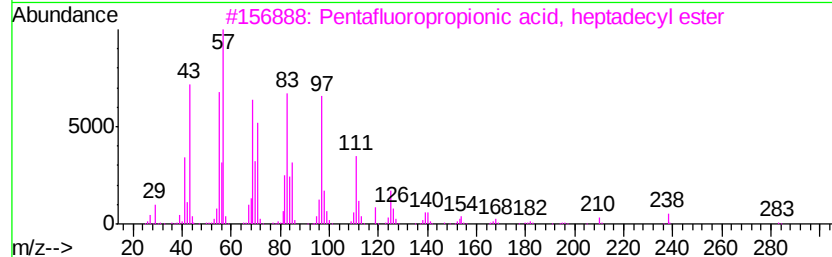
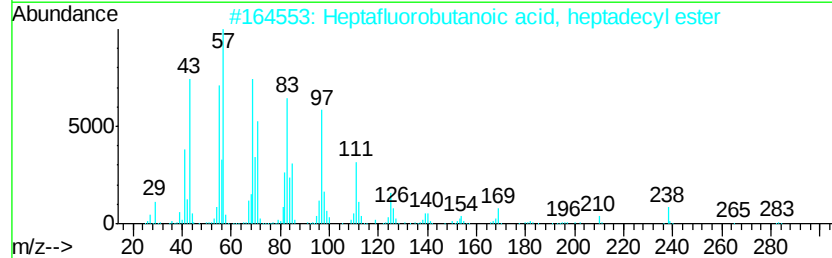
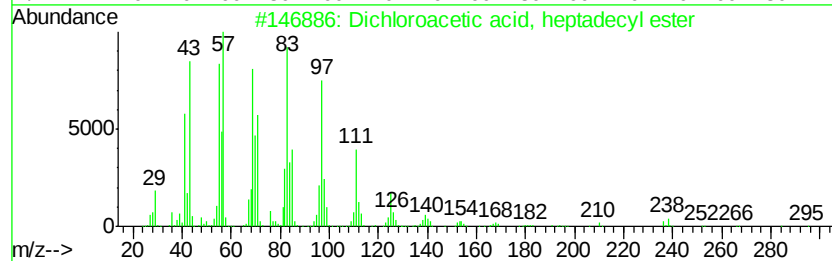
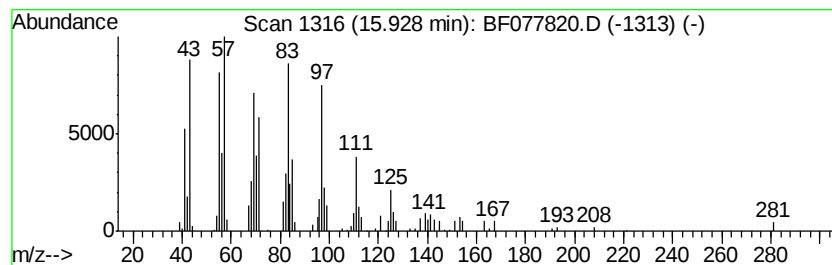
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Dichloroacetic acid, heptad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.93	4.52 ng	108239	Chrysene-d12	16.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	95
3		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	94
4		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



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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...	1.32	423.2	ng	4450940	1	7.16	210362	20.0
Butane, 2-methoxy...	1.61	6.1	ng	64566	1	7.16	210362	20.0
2-Pentanone, 4-hy...	4.93	11.5	ng	121315	1	7.16	210362	20.0
unknown6.88	6.88	72.5	ng	762894	1	7.16	210362	20.0
Dichloroacetic ac...	15.93	4.5	ng	108239	5	16.04	479125	20.0