

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031416\
 Data File : BF085435.D
 Acq On : 14 Mar 2016 18:10
 Operator : UM/SJ
 Sample : H1757-06
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TRACK-D-STOCKPICE-COMP2

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-BF030316.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	2.858	47	50	55	rVB	131147	205344	3.36%	0.469%
2	4.516	192	195	199	rBV	132612	201346	3.29%	0.460%
3	5.144	248	250	257	rVB	496497	790807	12.93%	1.806%
4	5.544	282	285	288	rVB	3414394	4270249	69.81%	9.754%
5	6.561	371	374	376	rBV	3531374	3804985	62.20%	8.692%
6	6.699	383	386	388	rBV	4404229	4627040	75.64%	10.570%
7	6.927	403	406	408	rBV	1042927	1003347	16.40%	2.292%
8	7.087	417	420	422	rVB	3662672	4124658	67.43%	9.422%
9	7.487	452	455	458	rBV	2727499	3076624	50.30%	7.028%
10	8.207	516	518	519	rBV	1583959	1340950	21.92%	3.063%
11	8.230	519	520	522	rVB	216734	166817	2.73%	0.381%
12	9.293	609	613	615	rBV	4656321	6116884	100.00%	13.973%
13	9.967	669	672	674	rBV	1475930	1491020	24.38%	3.406%
14	10.756	738	741	744	rBV	3305948	3429553	56.07%	7.834%
15	11.453	799	802	804	rBV	1300578	1470473	24.04%	3.359%
16	11.968	846	847	849	rBV	73041	68806	1.12%	0.157%
17	12.756	914	916	923	rVB	82209	94035	1.54%	0.215%
18	13.042	938	941	943	rBV	4862298	5422661	88.65%	12.387%
19	14.082	1030	1032	1035	rBV	876886	851771	13.92%	1.946%
20	15.545	1157	1160	1164	rBV	528291	797607	13.04%	1.822%
21	15.808	1177	1183	1185	rBV2	111641	422274	6.90%	0.965%

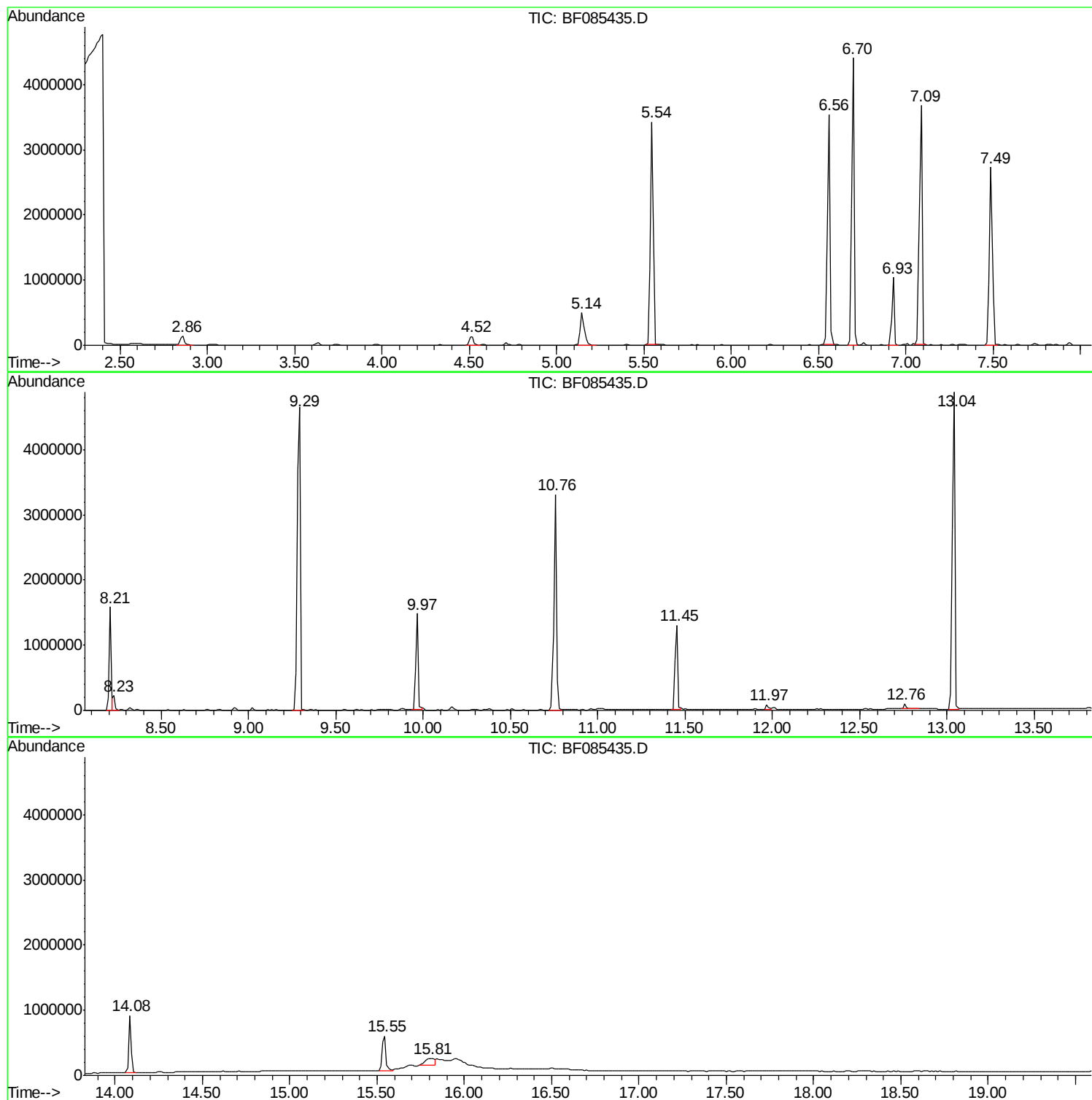
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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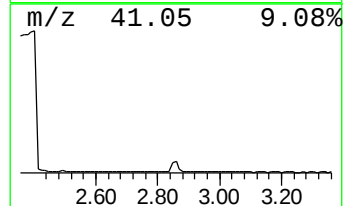
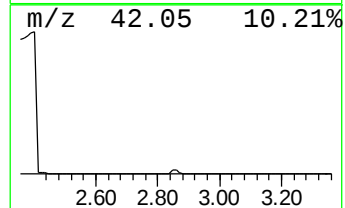
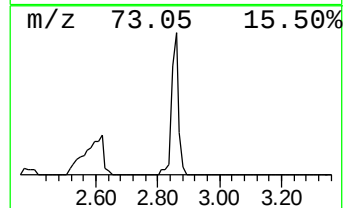
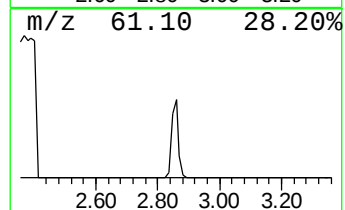
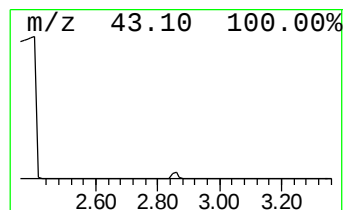
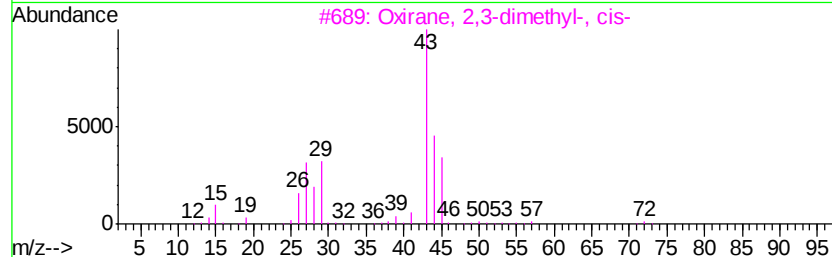
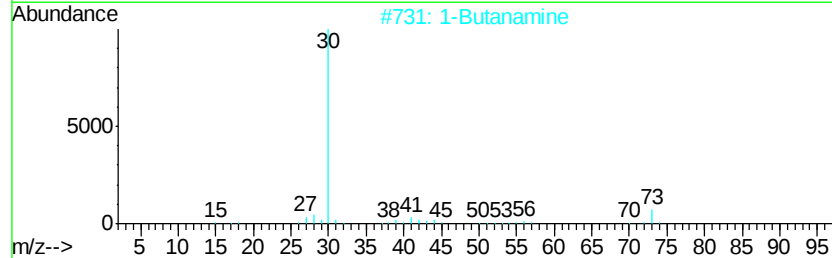
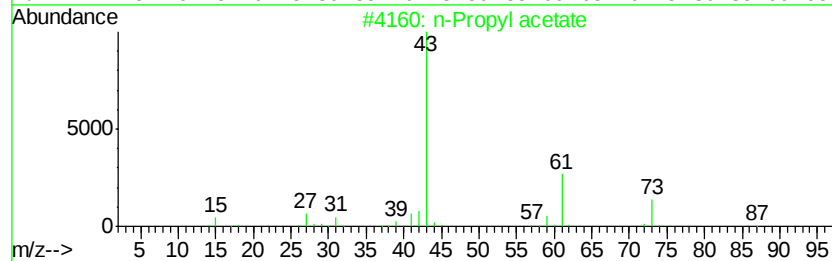
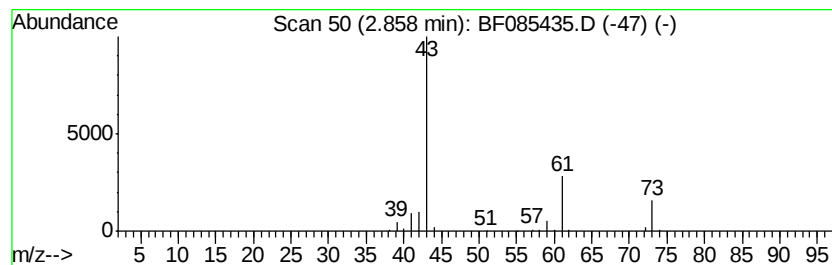
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	4.09 ng	205344	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		1-Butanamine	73	C4H11N	000109-73-9	7
3		Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5
4		Pentane	72	C5H12	000109-66-0	5
5		Ethanamine, N-ethyl-	73	C4H11N	000109-89-7	4



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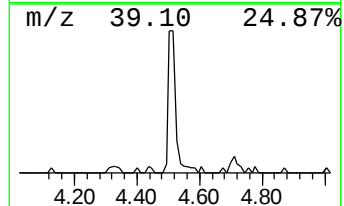
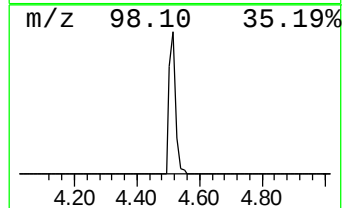
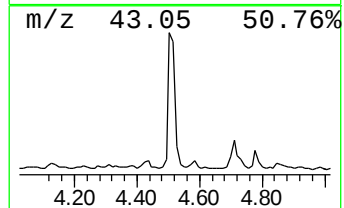
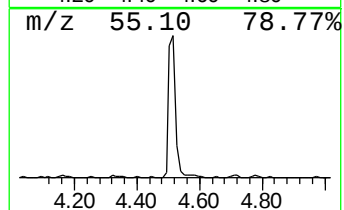
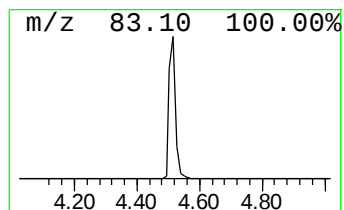
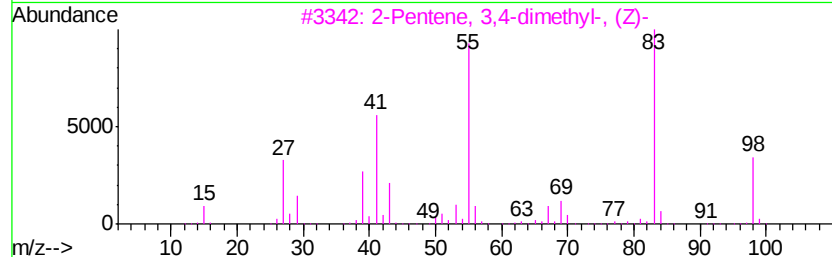
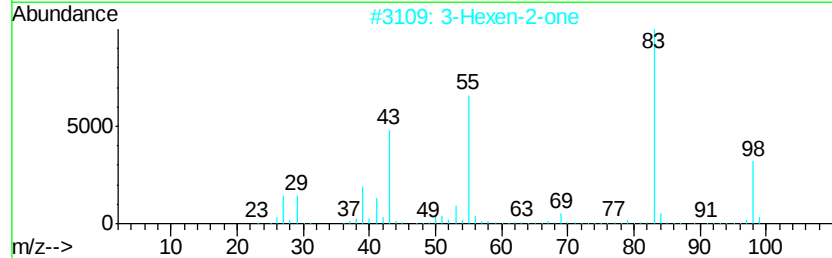
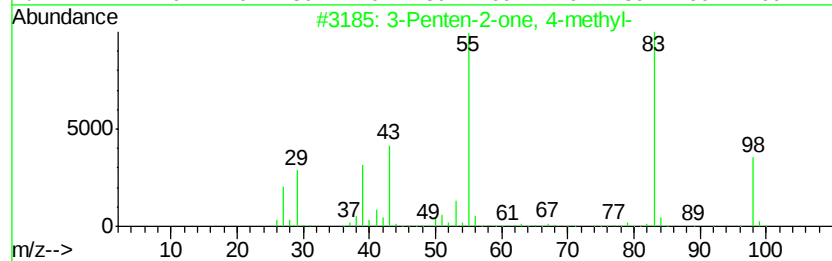
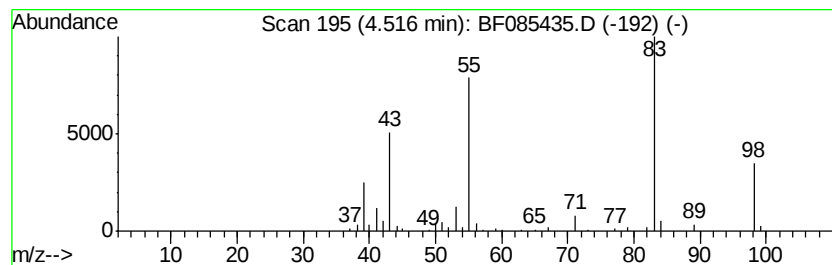
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	4.01 ng	201346	1,4-Dichlorobenzene-d4	6.93

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2			3-Hexen-2-one	98	C6H10O	000763-93-9	90
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	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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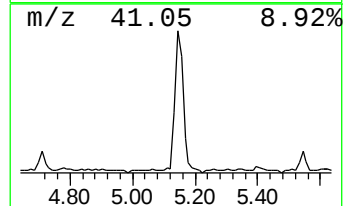
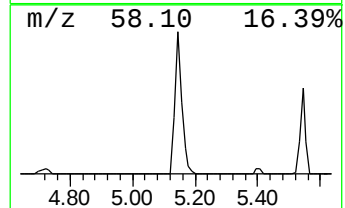
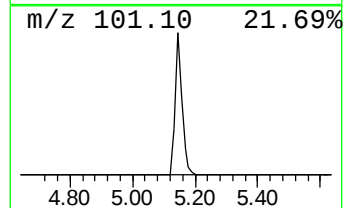
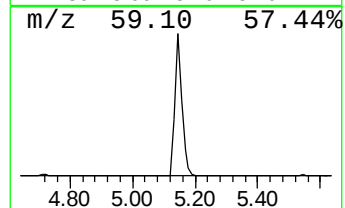
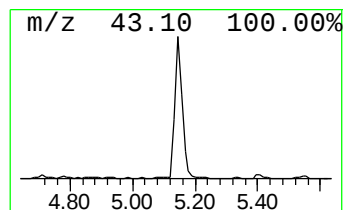
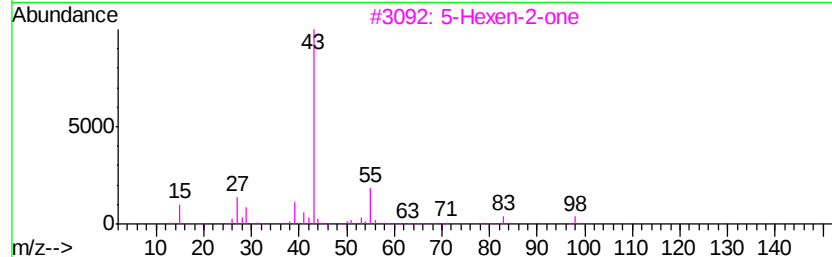
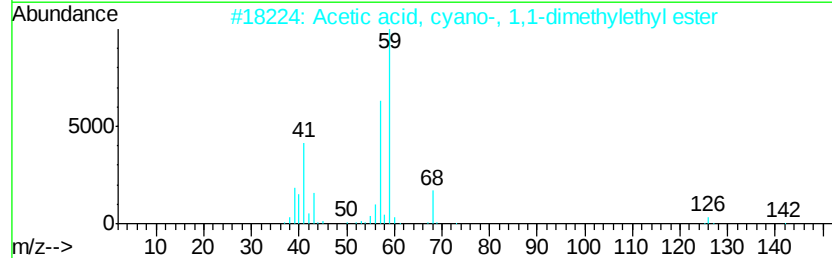
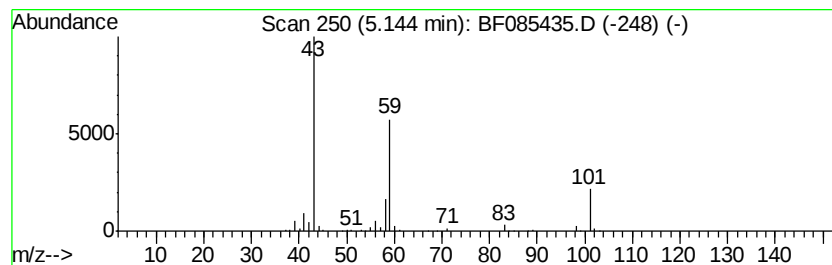
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	15.76 ng	790807	1,4-Dichlorobenzene-d4	6.93

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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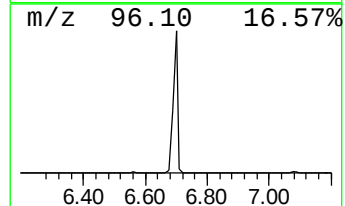
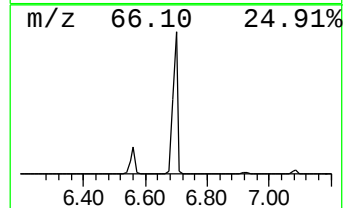
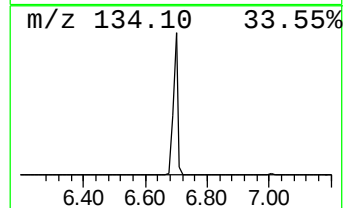
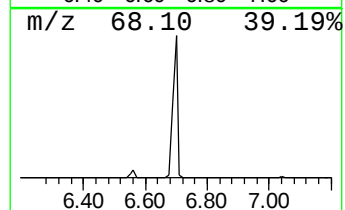
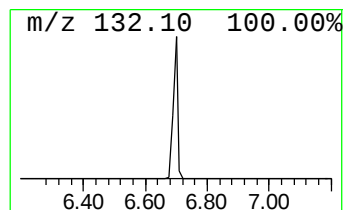
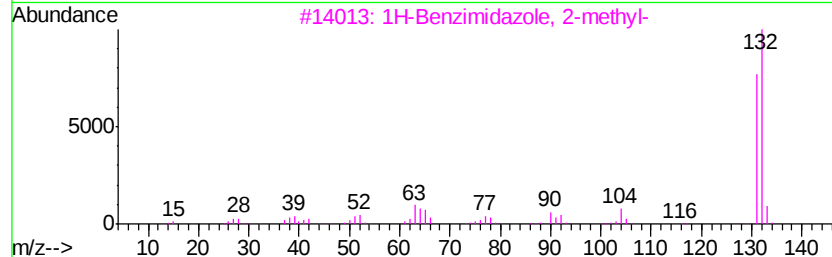
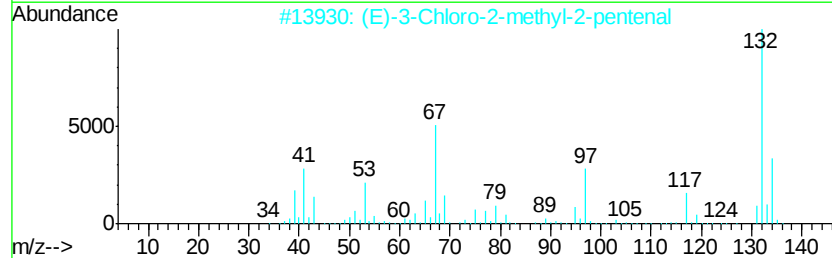
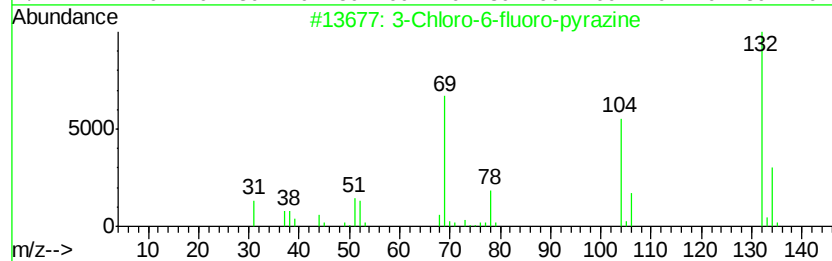
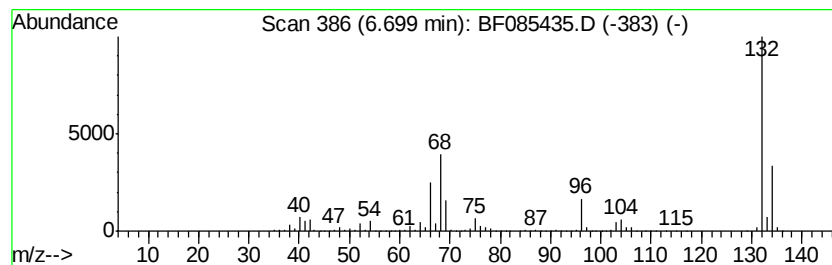
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	92.23 ng	4627040	1,4-Dichlorobenzene-d4	6.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
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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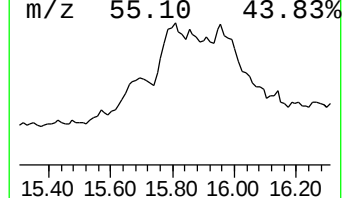
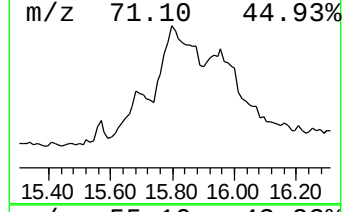
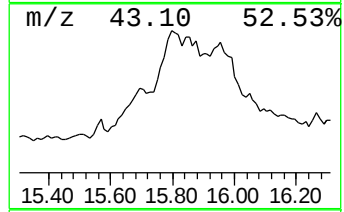
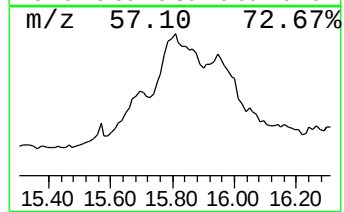
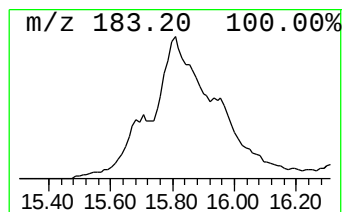
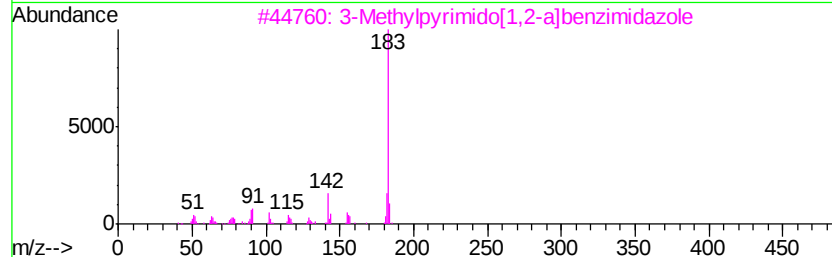
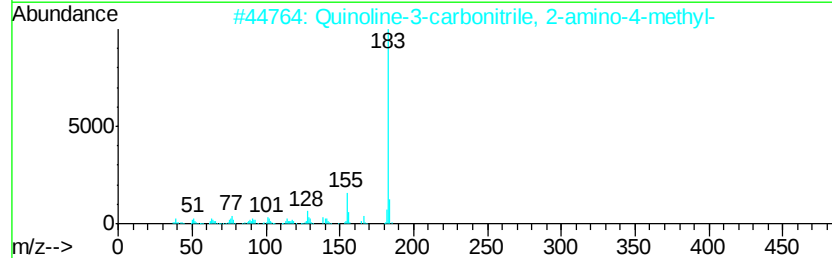
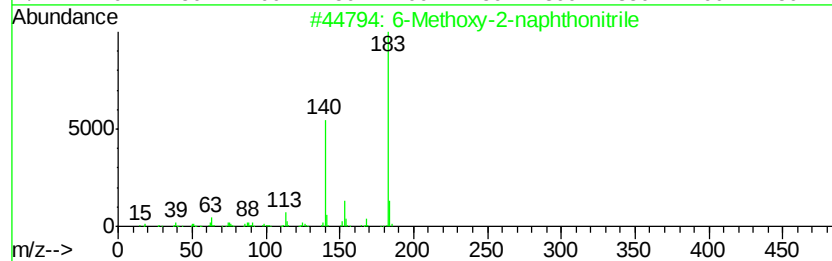
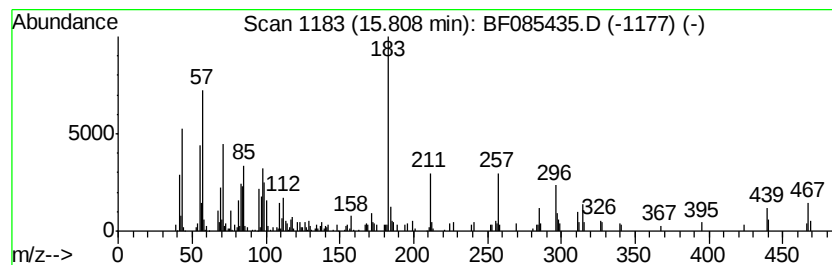
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Peak Number 6 unknown15.81 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	10.59 ng	422274	Perylene-d12	15.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Methoxy-2-naphthonitrile	183	C12H9NO	067886-70-8	38
2		Quinoline-3-carbonitrile, 2-amin...	183	C11H9N3	028448-11-5	38
3		3-Methylpyrimido[1,2-a]benzimid...	183	C11H9N3	085495-17-6	38
4		Benzenamine, N-methyl-N-phenyl-	183	C13H13N	000552-82-9	35
5		5-Amino-3-methyl-thiophene-2,4-d...	257	C11H15N04S	303101-08-8	35



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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	2.86	4.1	ng	205344	1	6.93	1003350	20.0
3-Penten-2-one, 4...	4.52	4.0	ng	201346	1	6.93	1003350	20.0
2-Pentanone, 4-hy...	5.14	15.8	ng	790807	1	6.93	1003350	20.0
unknown6.70	6.70	92.2	ng	4627040	1	6.93	1003350	20.0
unknown15.81	15.81	10.6	ng	422274	6	15.55	797607	20.0