

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093638.D
 Acq On : 14 Mar 2017 5:44
 Operator : SJ/MA
 Sample : I2199-30
 Misc :
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-111

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-BF030717.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	2.458	48	50	60	rVB	43005	135130	2.21%	0.268%
2	3.144	107	110	124	rBV	99179	308072	5.04%	0.611%
3	4.184	200	201	214	rVB	274923	629186	10.30%	1.247%
4	4.870	259	261	278	rBV	936198	1881630	30.80%	3.729%
5	5.316	298	300	325	rBV	4197989	5978798	97.86%	11.848%
6	5.716	333	335	348	rVB	57081	116396	1.91%	0.231%
7	6.367	390	392	400	rBV	3593139	5341738	87.44%	10.586%
8	6.482	400	402	405	rVB	5162363	5201392	85.14%	10.308%
9	6.710	420	422	431	rVB	966297	1146378	18.76%	2.272%
10	6.859	433	435	438	rBV	4158118	4174827	68.34%	8.273%
11	7.282	470	472	488	rBV	3257148	3884020	63.58%	7.697%
12	8.002	533	535	547	rBV	1242805	1504970	24.63%	2.982%
13	9.076	626	629	632	rBV	4336334	6109256	100.00%	12.107%
14	9.751	686	688	691	rBV	1111849	1635638	26.77%	3.241%
15	10.551	756	758	761	rBV2	2489983	3234258	52.94%	6.409%
16	11.248	816	819	825	rBV	1675502	1664772	27.25%	3.299%
17	12.837	955	958	961	rBV	4619544	5287490	86.55%	10.478%
18	13.900	1049	1051	1061	rVB	919108	1346832	22.05%	2.669%
19	15.305	1171	1174	1183	rBV	533135	880829	14.42%	1.746%

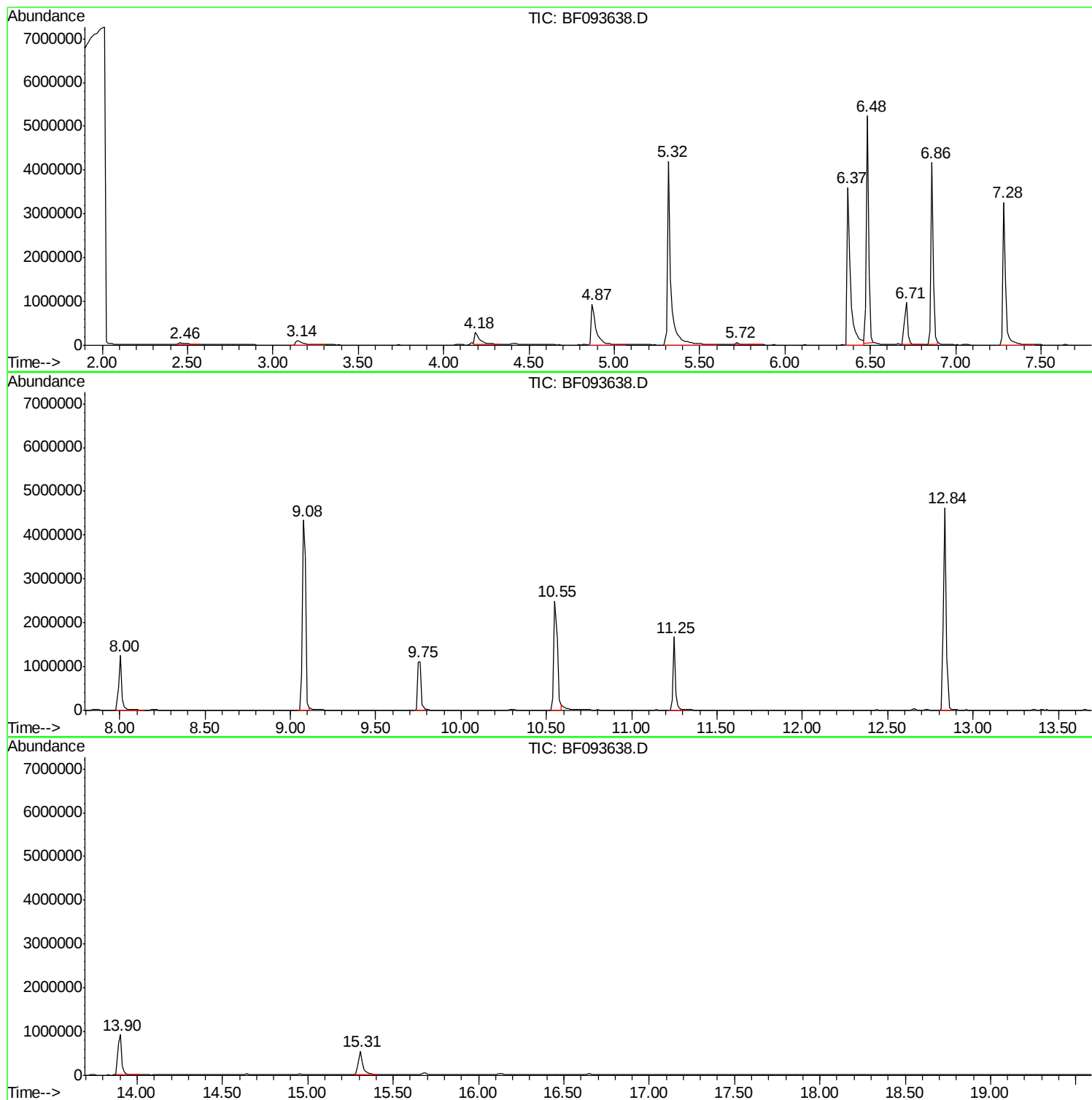
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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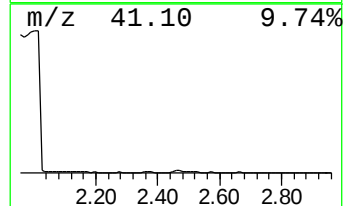
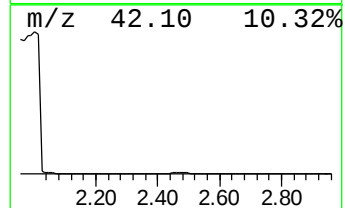
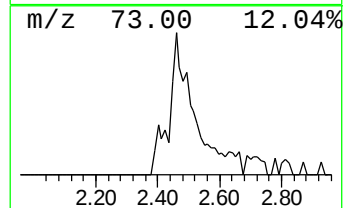
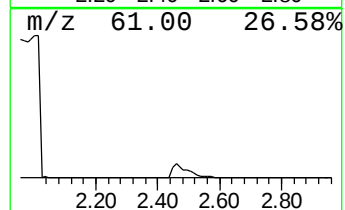
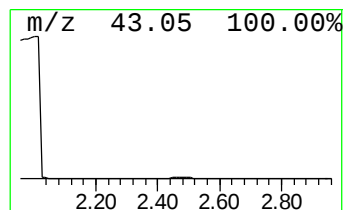
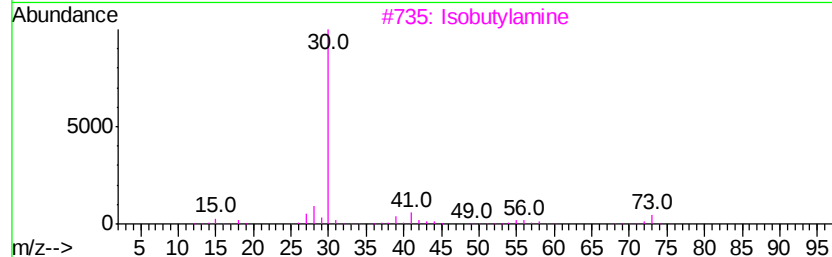
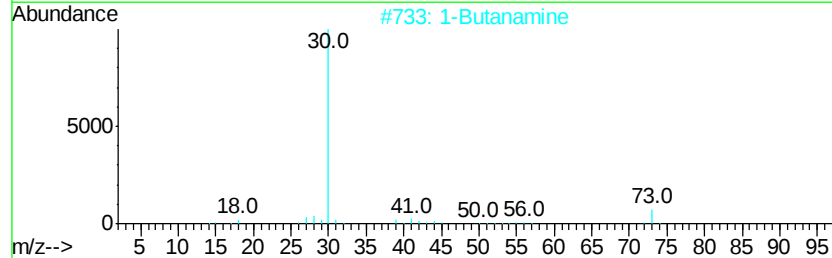
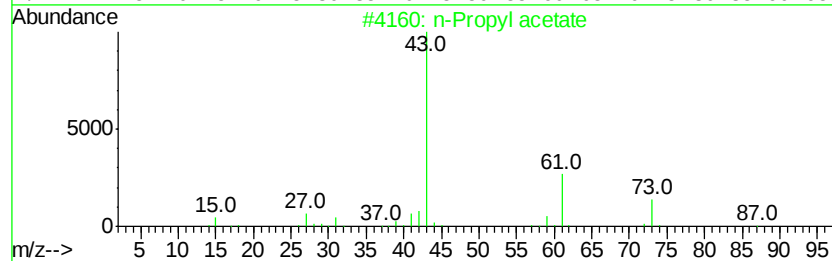
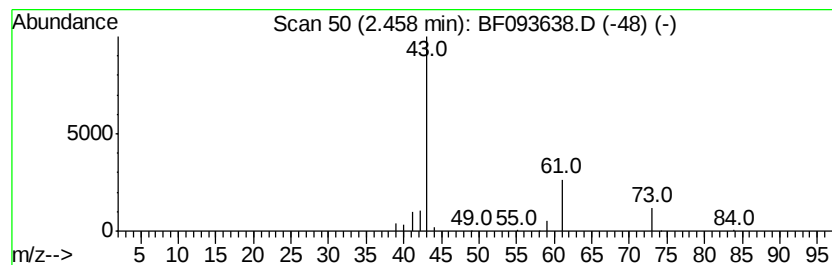
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
2.46	2.36 ng	135130	1,4-Dichlorobenzene-d4	6.71	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	1-Butanamine	73	C4H11N	000109-73-9	3
3	Isobutylamine	73	C4H11N	000078-81-9	3
4	Methane, nitro-	61	CH3NO2	000075-52-5	3
5	Hydrogen azide	43	HN3	007782-79-8	3



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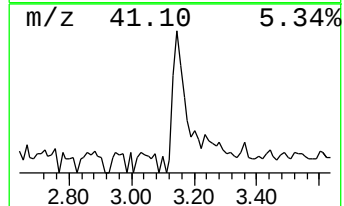
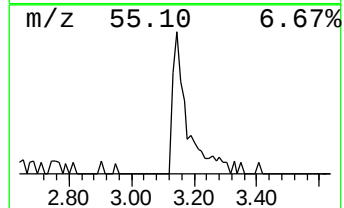
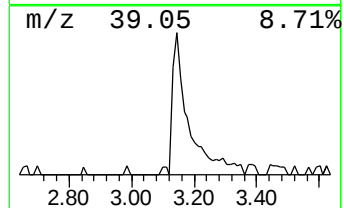
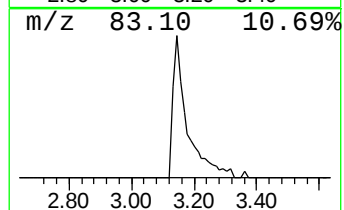
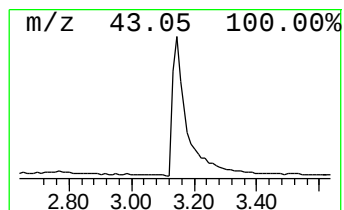
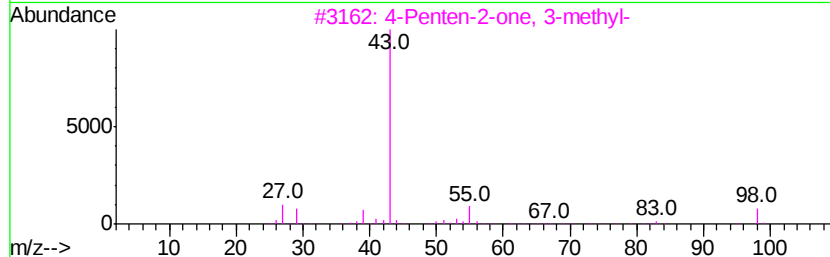
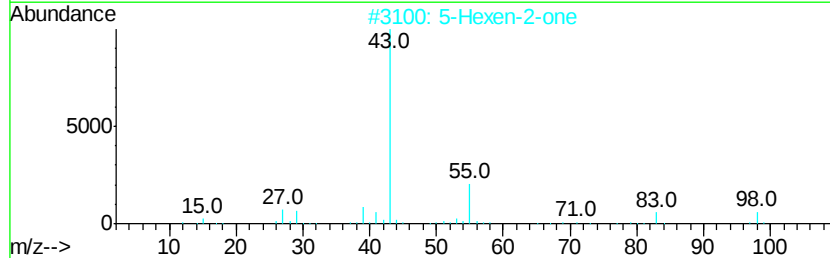
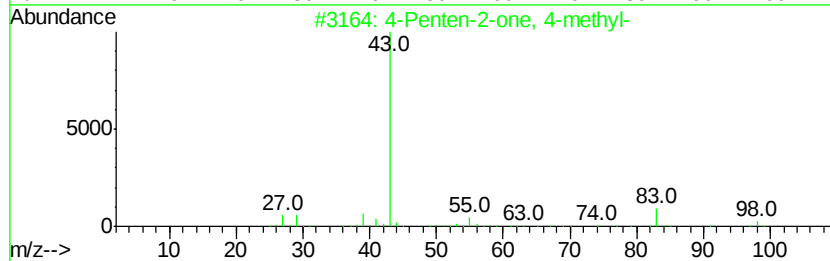
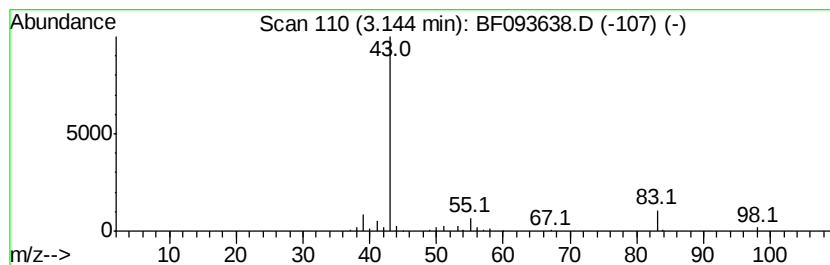
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	5.37 ng	308072	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	86
2		5-Hexen-2-one	98	C6H10O	000109-49-9	32
3		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	32
4		Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	10
5		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9



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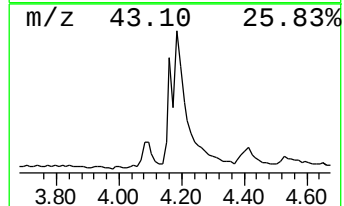
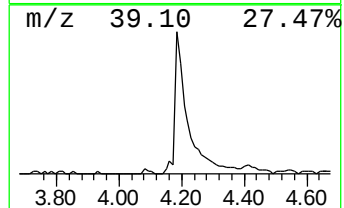
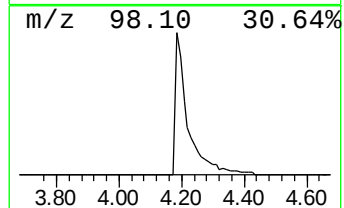
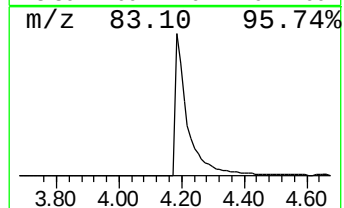
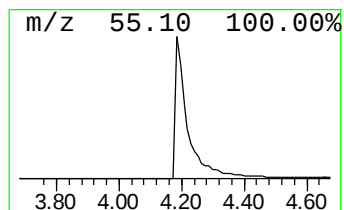
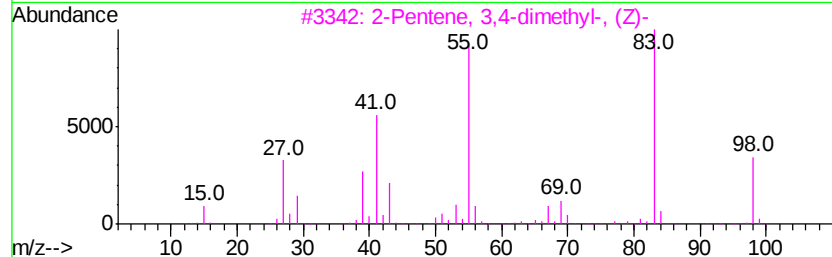
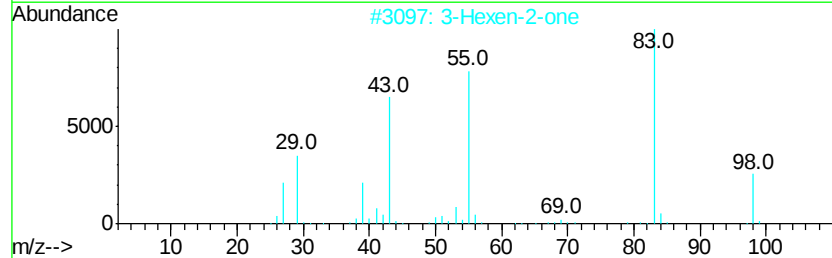
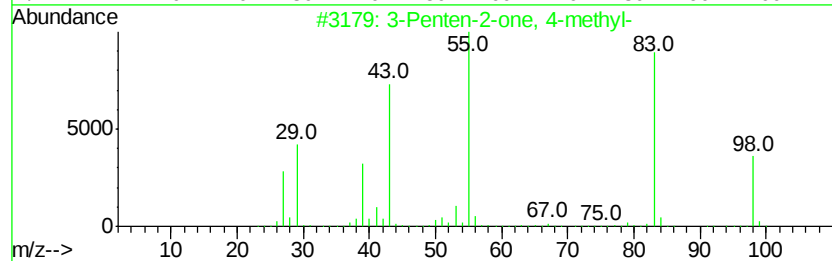
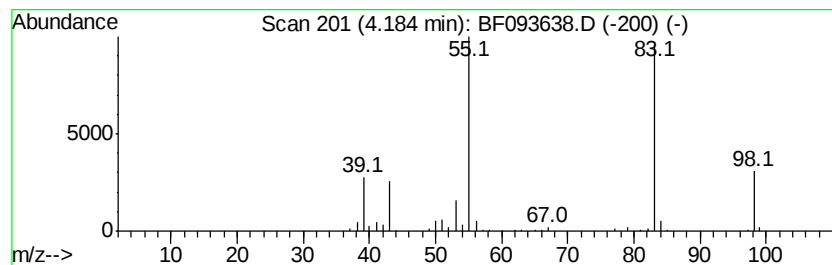
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Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	10.98 ng	629186	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5		Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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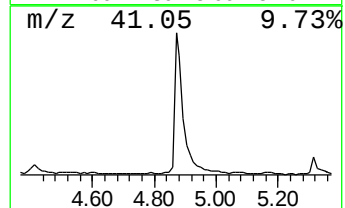
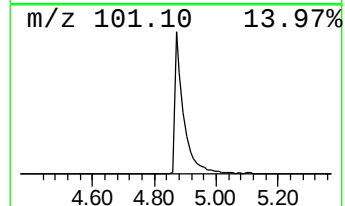
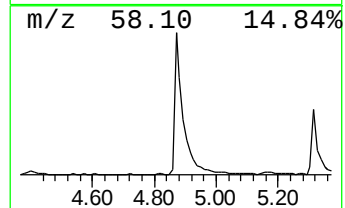
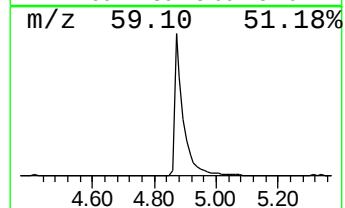
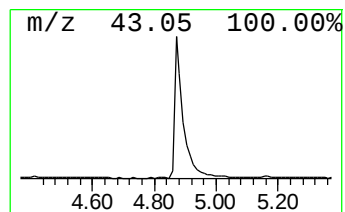
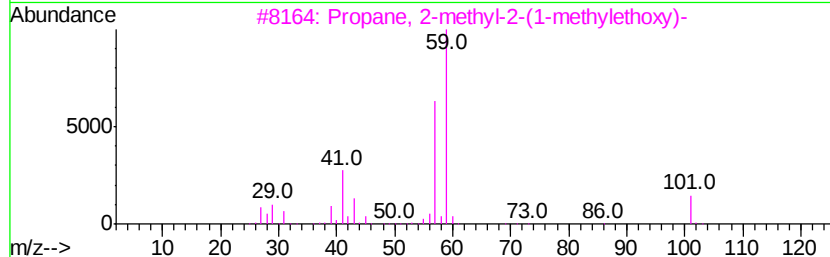
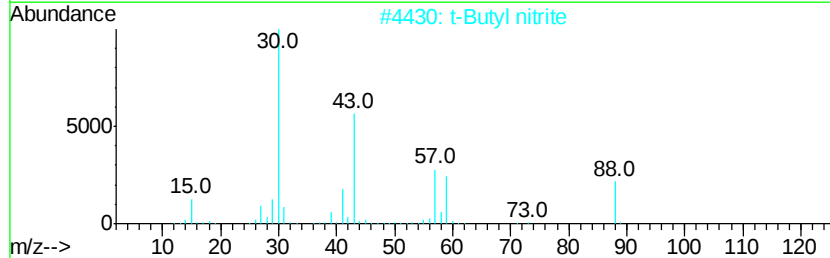
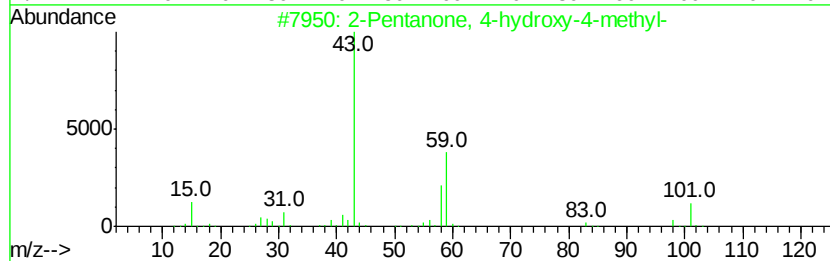
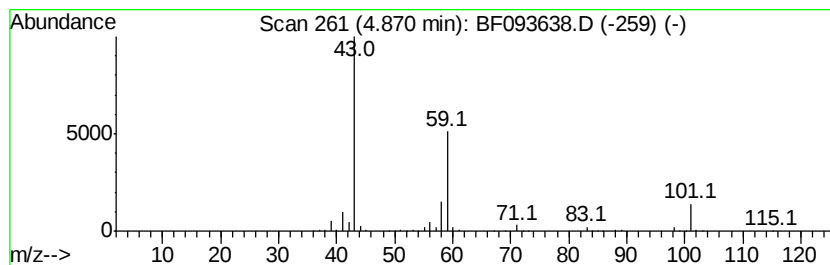
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	32.83 ng	1881630	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
3		Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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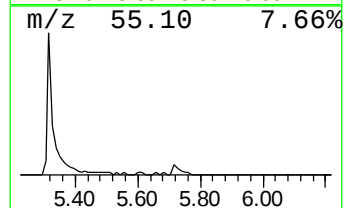
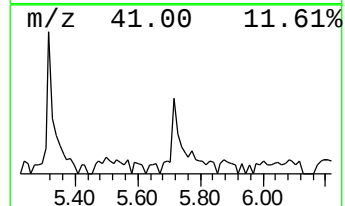
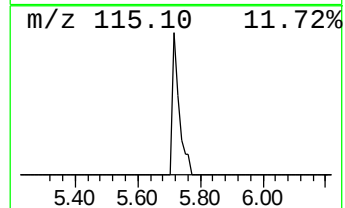
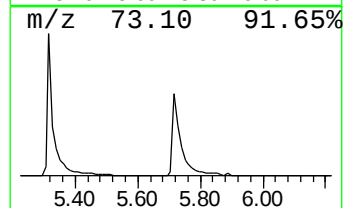
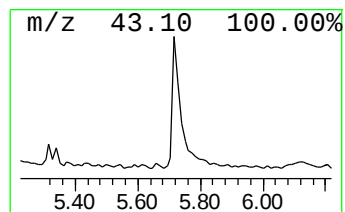
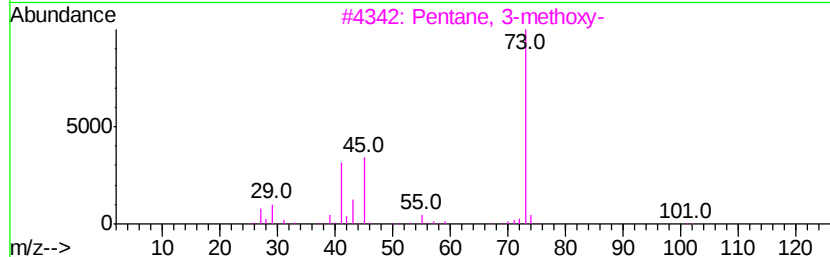
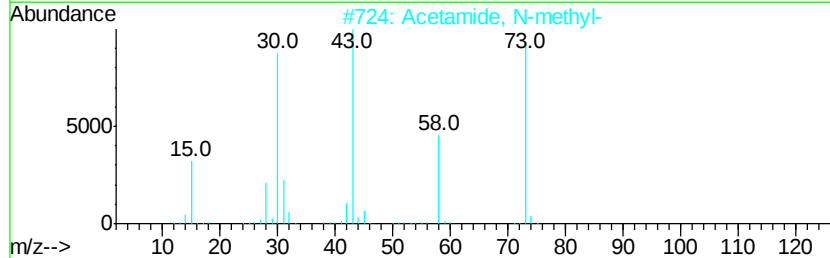
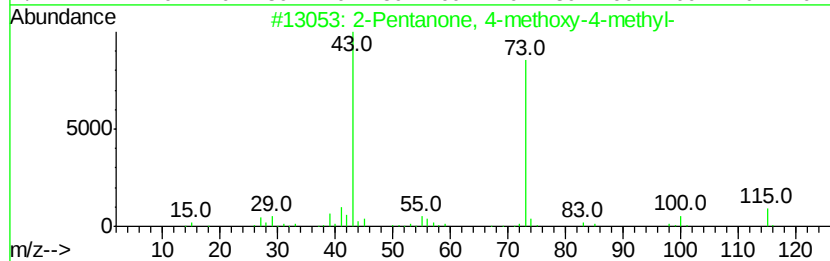
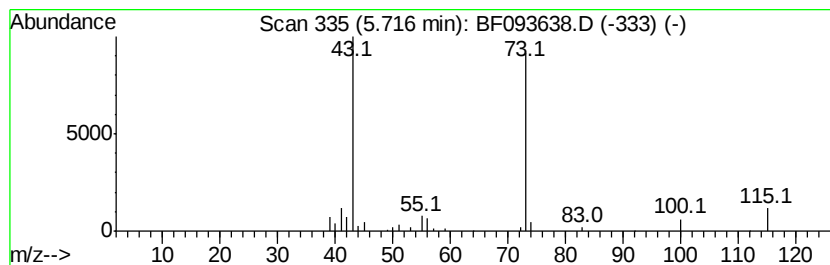
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.03 ng	116396	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	49
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		N-Ethylformamide	73	C3H7NO	000627-45-2	10
5		Guanidine, methyl-	73	C2H7N3	000471-29-4	9



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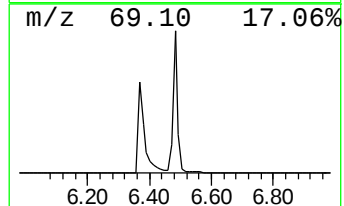
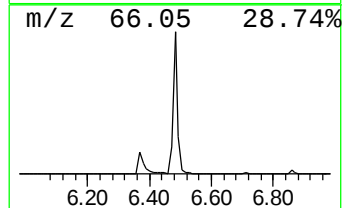
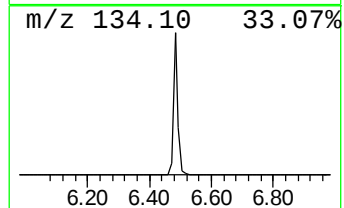
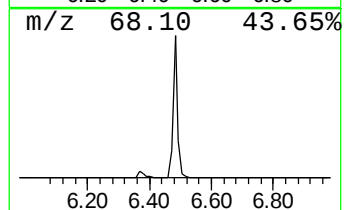
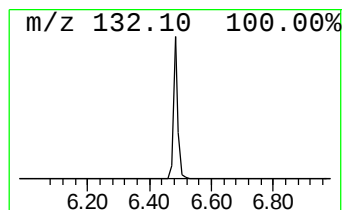
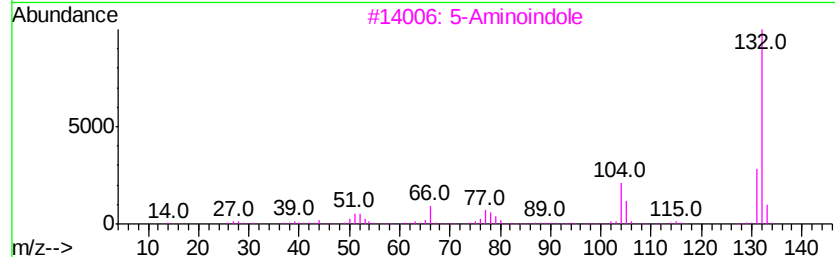
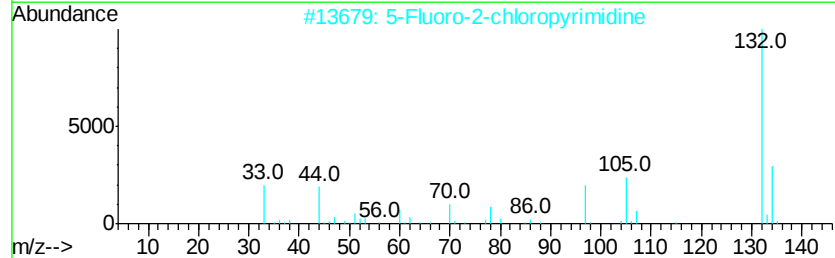
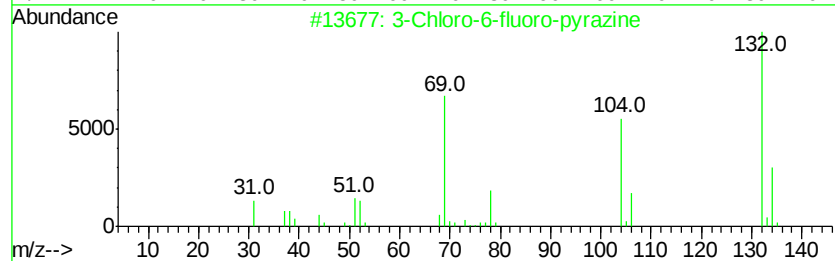
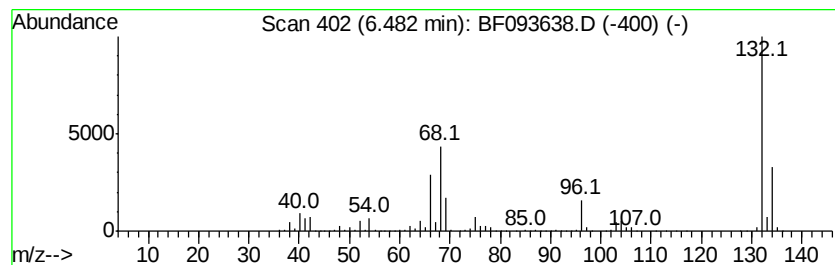
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TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	90.74 ng	5201390	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093638.D
Acq On : 14 Mar 2017 5:44
Operator : SJ/MA
Sample : I2199-30
Misc :
ALS Vial : 38 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-111

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	2.46	2.4	ng	135130	1	6.71	1146380	20.0
4-Penten-2-one, 4...	3.14	5.4	ng	308072	1	6.71	1146380	20.0
3-Penten-2-one, 4...	4.18	11.0	ng	629186	1	6.71	1146380	20.0
2-Pentanone, 4-hy...	4.87	32.8	ng	1881630	1	6.71	1146380	20.0
2-Pentanone, 4-me...	5.72	2.0	ng	116396	1	6.71	1146380	20.0
unknown6.48	6.48	90.7	ng	5201390	1	6.71	1146380	20.0