

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
 Data File : BF085268.D
 Acq On : 8 Mar 2016 21:10
 Operator : UM/SJ
 Sample : H1707-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RW-48-S2-GRID5

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-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	2.344	3	5	7	rVB	4553293	6208772	100.00%	13.293%
2	2.881	49	52	56	rVB	143628	223034	3.59%	0.478%
3	3.670	119	121	125	rVB	74902	111394	1.79%	0.239%
4	4.550	195	198	201	rBV	283303	356163	5.74%	0.763%
5	5.179	250	253	260	rVB	528131	945165	15.22%	2.024%
6	5.579	284	288	290	rBV	3374135	4194966	67.57%	8.982%
7	6.584	373	376	378	rBV	3312412	3325935	53.57%	7.121%
8	6.733	386	389	391	rBV	3766112	4465065	71.92%	9.560%
9	6.962	406	409	411	rBV	1077586	923153	14.87%	1.977%
10	7.122	420	423	425	rVB	3523694	3689819	59.43%	7.900%
11	7.522	455	458	460	rBV	2771402	2735704	44.06%	5.857%
12	8.242	519	521	525	rBV2	1356081	1515340	24.41%	3.244%
13	9.328	612	616	618	rBV	3688020	5200405	83.76%	11.134%
14	10.002	672	675	677	rBV	1383657	1291949	20.81%	2.766%
15	10.791	741	744	746	rBV	3070626	3165573	50.99%	6.778%
16	11.488	802	805	807	rBV	1317573	1355431	21.83%	2.902%
17	13.076	941	944	946	rBV	4399577	5306098	85.46%	11.361%
18	14.117	1033	1035	1038	rBV	1186078	1061874	17.10%	2.274%
19	15.580	1160	1163	1166	rBV	459861	629533	10.14%	1.348%

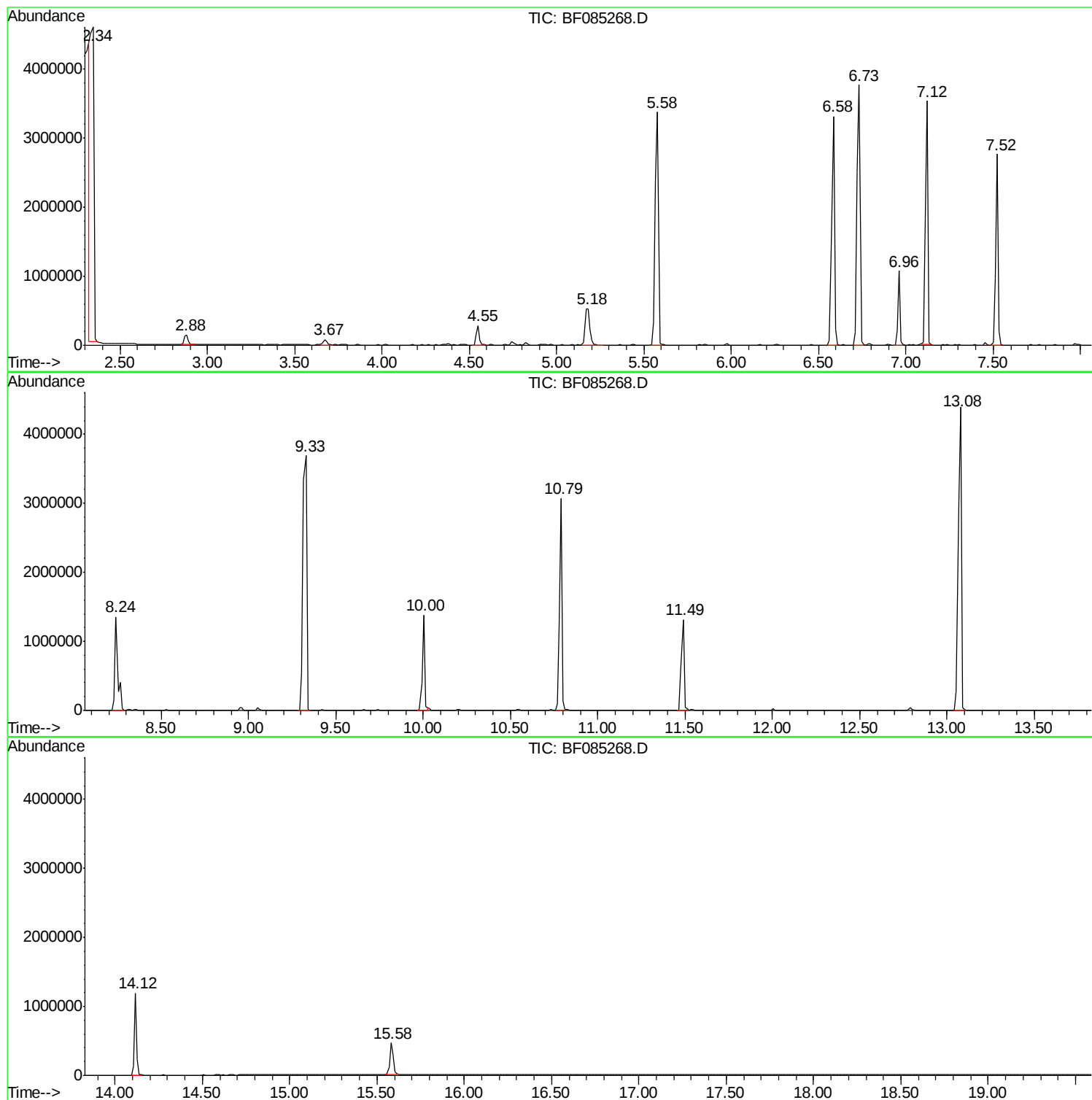
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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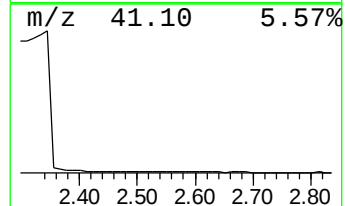
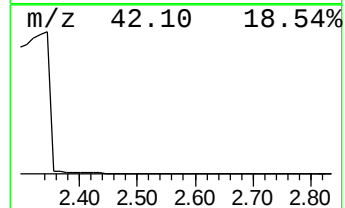
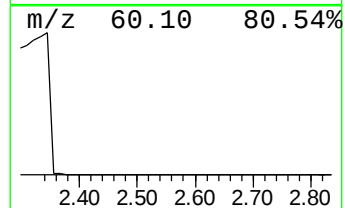
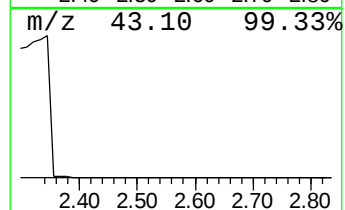
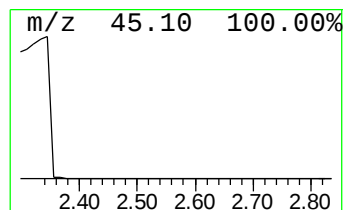
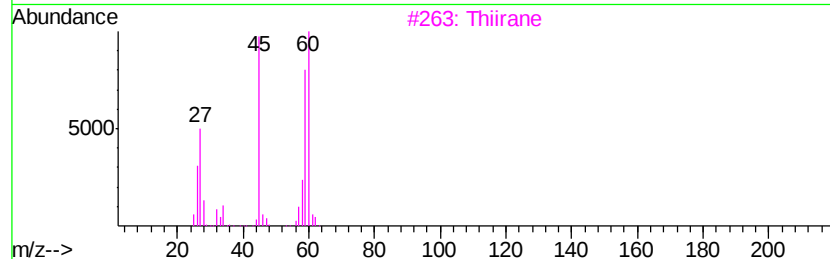
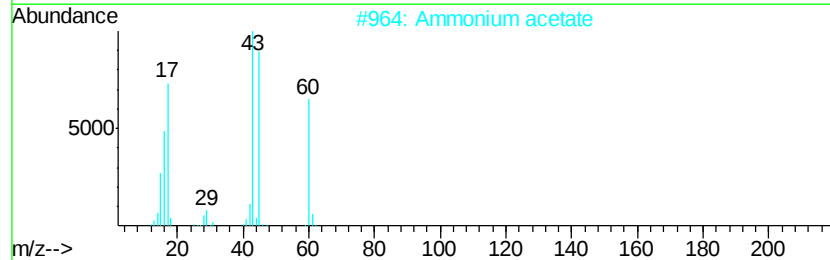
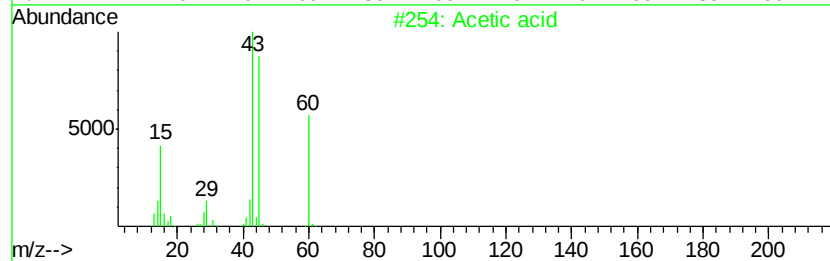
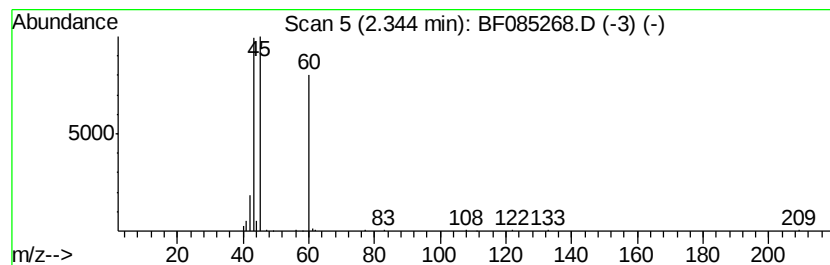
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.34	134.51 ng	6208770	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid	60	C2H4O2	000064-19-7	90
2		Ammonium acetate	77	C2H7NO2	000631-61-8	64
3		Thiirane	60	C2H4S	000420-12-2	9
4		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5		Carbonyl sulfide	60	COS	000463-58-1	5



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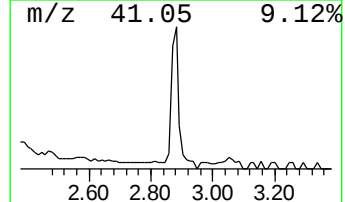
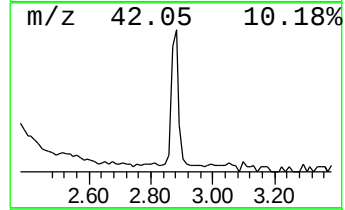
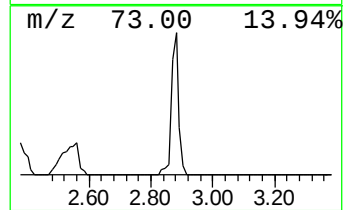
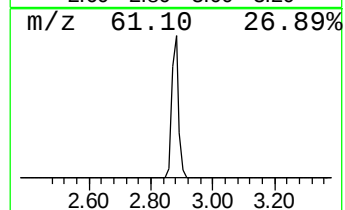
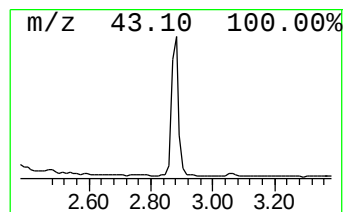
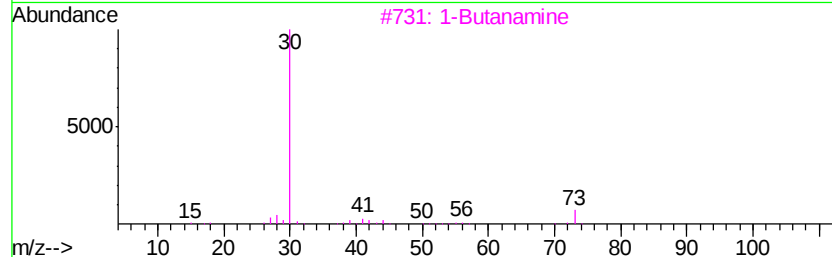
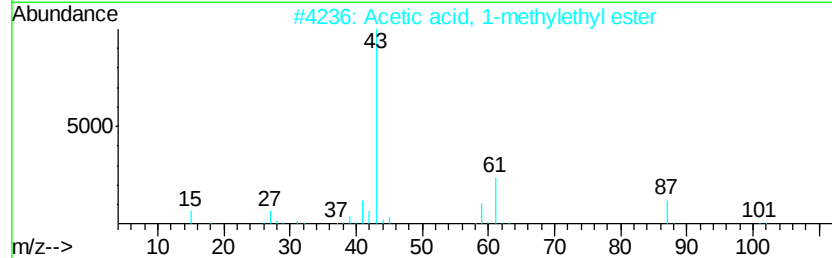
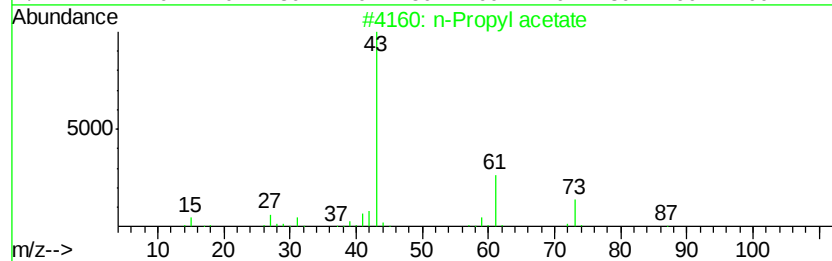
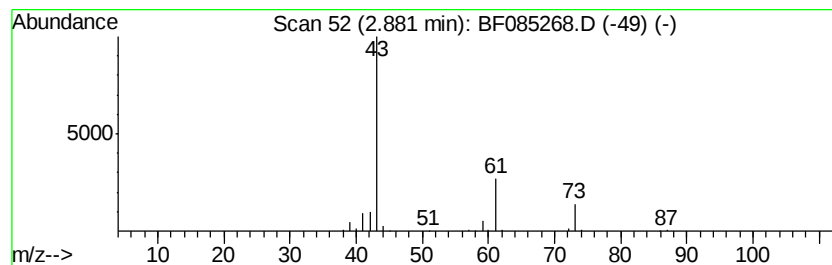
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Peak Number 2 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	4.83 ng	223034	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Acetic acid, 1-methylethyl ester	102	C5H10O2	000108-21-4	38
3		1-Butanamine	73	C4H11N	000109-73-9	7
4		Isobutylamine	73	C4H11N	000078-81-9	5
5		Pentane	72	C5H12	000109-66-0	5



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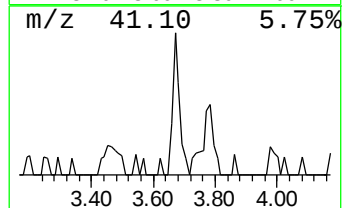
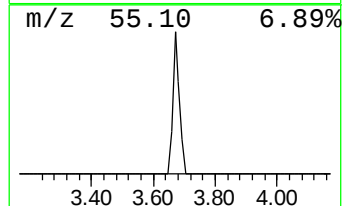
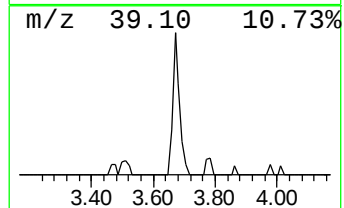
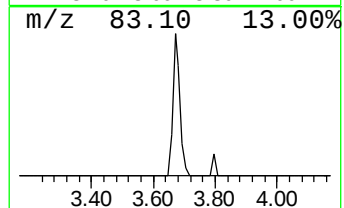
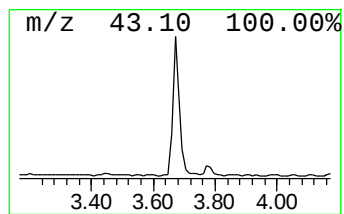
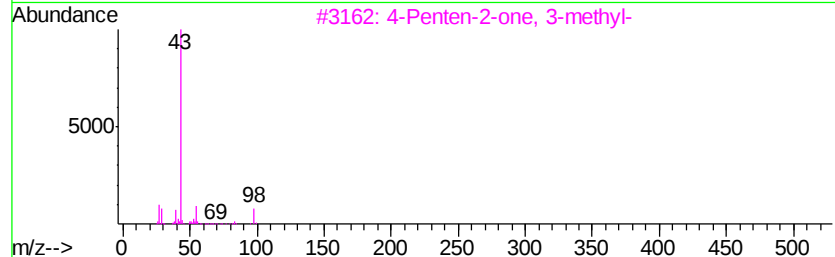
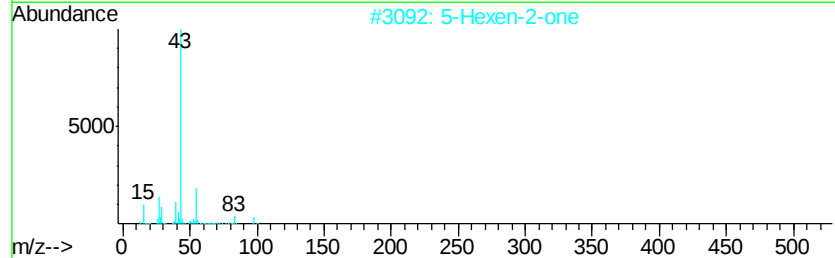
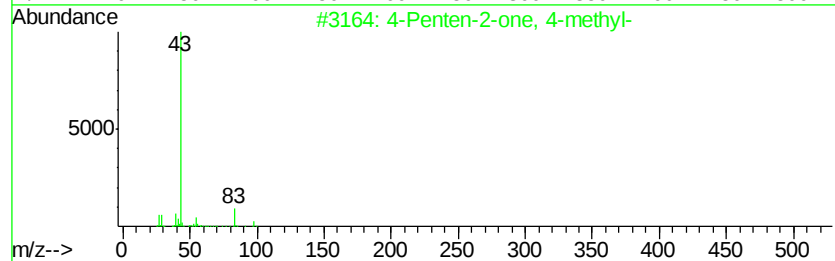
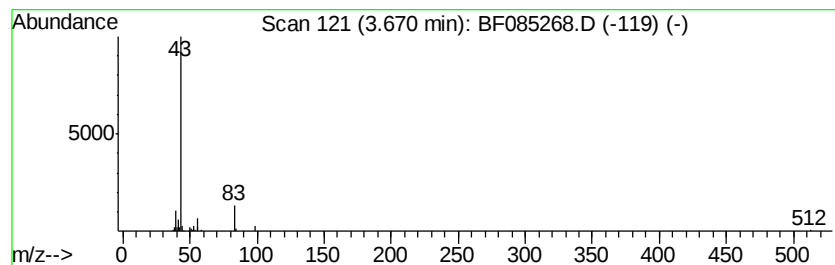
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Peak Number 3 4-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.67	2.41 ng	111394	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2			5-Hexen-2-one	98	C6H10O	000109-49-9	50
3			4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	50
4			2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	23
5			Isoxazole, 5-methyl-	83	C4H5NO	005765-44-6	9



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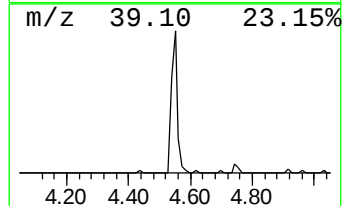
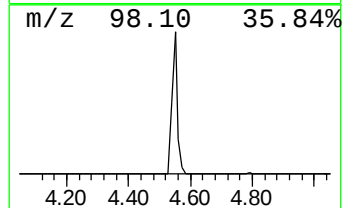
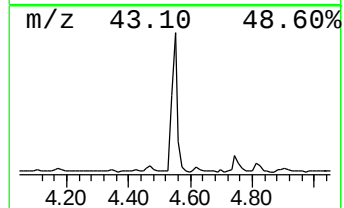
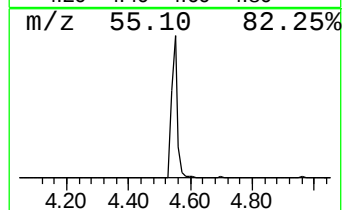
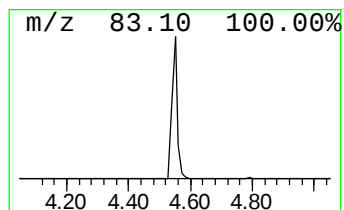
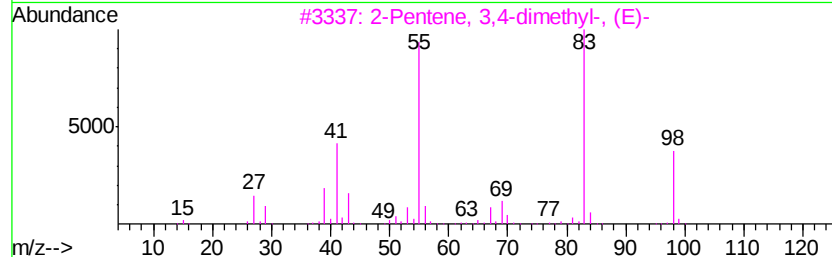
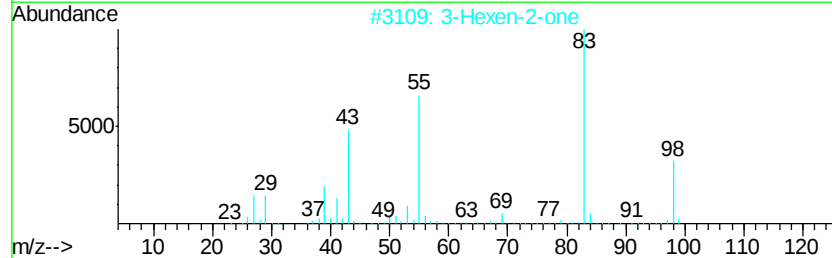
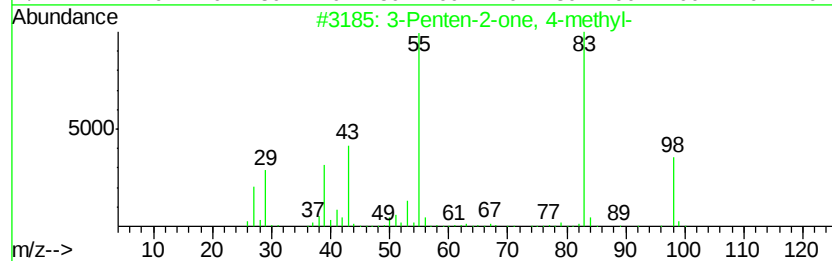
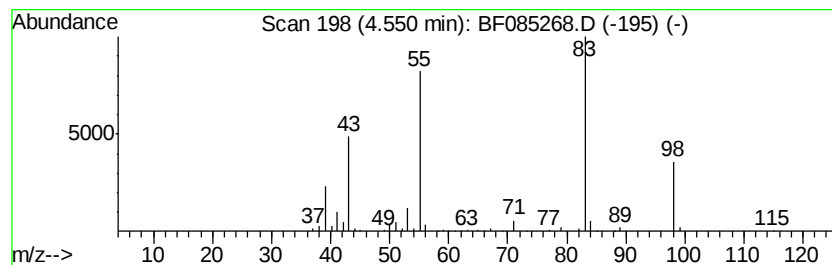
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Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	7.72 ng	356163	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			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-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	86



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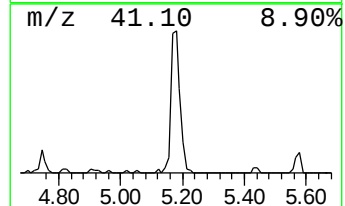
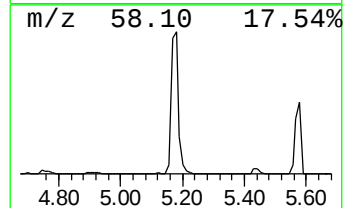
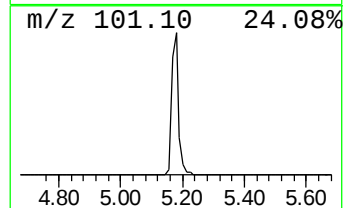
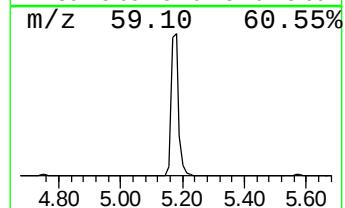
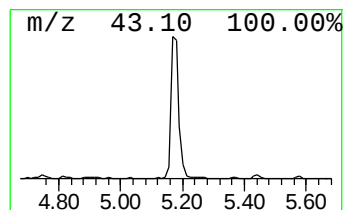
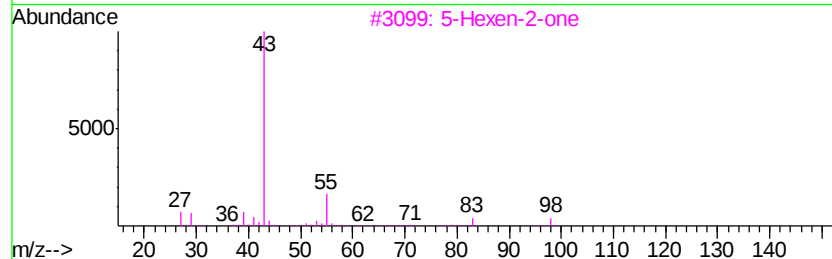
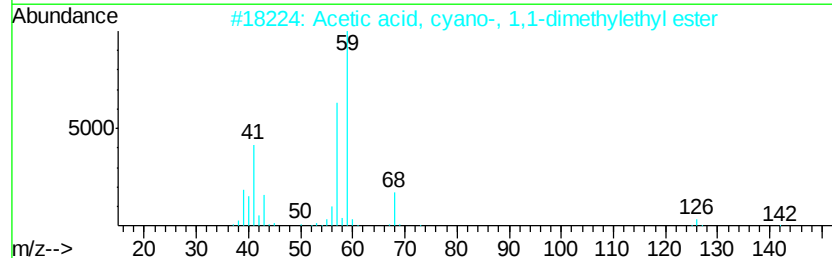
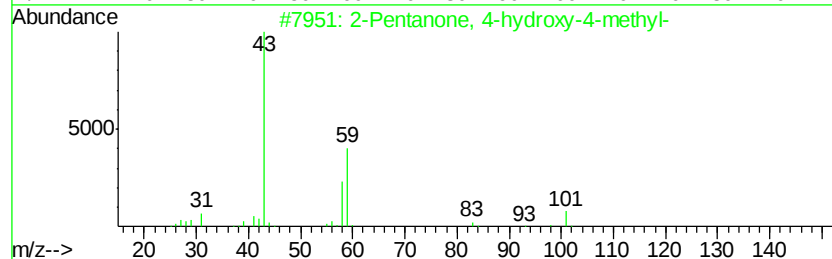
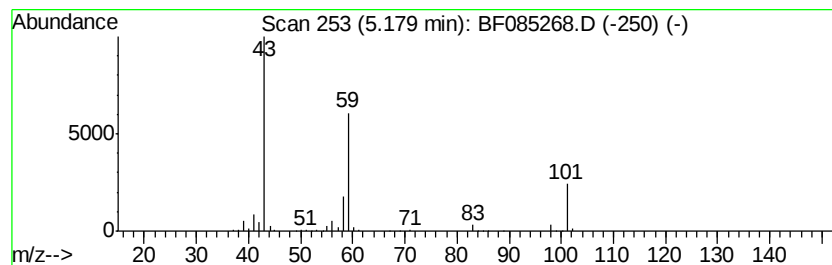
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	20.48 ng	945165	1,4-Dichlorobenzene-d4	6.96

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	17
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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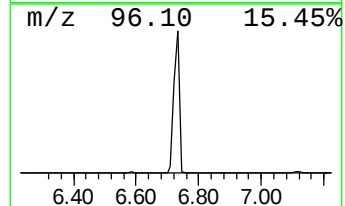
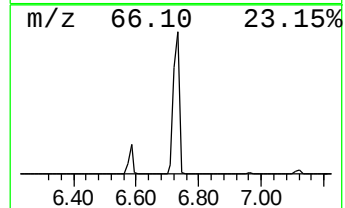
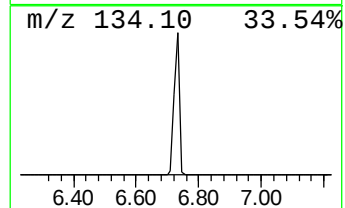
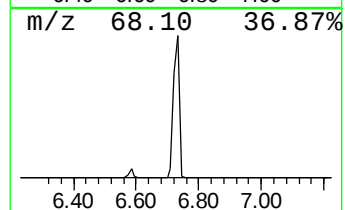
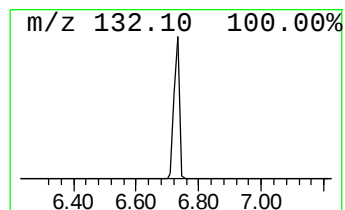
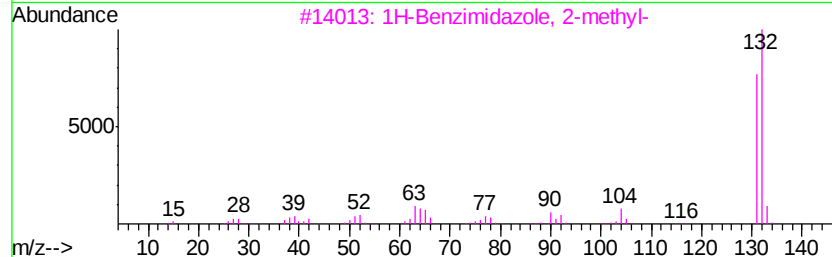
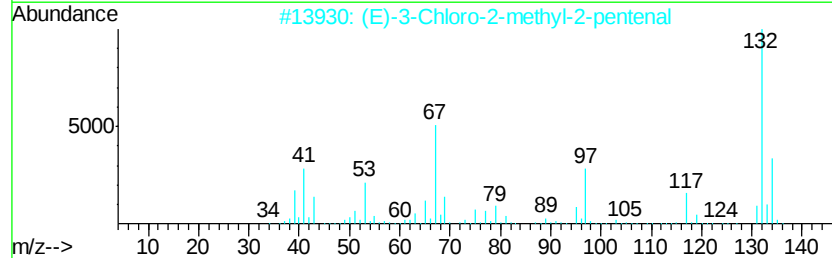
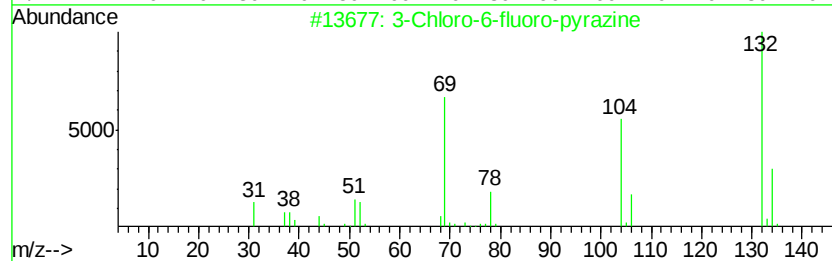
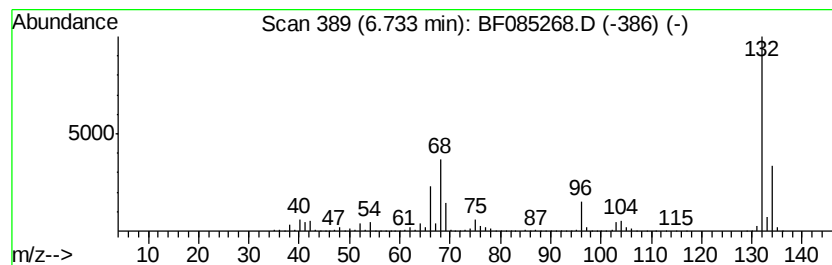
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	96.74 ng	4465070	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4			Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030816\
Data File : BF085268.D
Acq On : 8 Mar 2016 21:10
Operator : UM/SJ
Sample : H1707-05
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RW-48-S2-GRID5

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid	2.34	134.5	ng	6208770	1	6.96	923153	20.0
n-Propyl acetate	2.88	4.8	ng	223034	1	6.96	923153	20.0
4-Penten-2-one, 4...	3.67	2.4	ng	111394	1	6.96	923153	20.0
3-Penten-2-one, 4...	4.55	7.7	ng	356163	1	6.96	923153	20.0
2-Pentanone, 4-hy...	5.18	20.5	ng	945165	1	6.96	923153	20.0
unknown6.73	6.73	96.7	ng	4465070	1	6.96	923153	20.0