

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093635.D
 Acq On : 14 Mar 2017 4:21
 Operator : SJ/MA
 Sample : I2199-27
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-105

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	65	rVB	127905	302291	4.70%	0.583%
2	3.144	107	110	132	rVB	197606	483583	7.52%	0.933%
3	4.184	197	201	218	rBV2	355144	1044976	16.26%	2.016%
4	4.402	218	220	224	rBV	81601	149689	2.33%	0.289%
5	4.882	260	262	278	rBV	899323	1907727	29.68%	3.680%
6	5.316	298	300	325	rBV	4235992	6177422	96.10%	11.916%
7	5.716	333	335	345	rVB	55068	105360	1.64%	0.203%
8	6.367	391	392	400	rBV2	3246635	5493605	85.46%	10.597%
9	6.482	400	402	405	rVB	4976914	5211788	81.08%	10.053%
10	6.710	420	422	430	rVB	1055580	1143026	17.78%	2.205%
11	6.859	433	435	438	rBV	3931888	4238717	65.94%	8.176%
12	7.282	470	472	475	rBV	3076704	3741193	58.20%	7.217%
13	8.002	533	535	544	rBV	1357148	1520279	23.65%	2.933%
14	9.088	627	630	632	rBV	4648282	6428049	100.00%	12.400%
15	9.762	686	689	691	rBV	1357756	1603653	24.95%	3.093%
16	10.562	756	759	761	rBV	2296650	3348726	52.10%	6.460%
17	11.248	817	819	824	rBV	1681020	1668732	25.96%	3.219%
18	12.837	955	958	961	rBV	4520826	5204077	80.96%	10.039%
19	13.900	1049	1051	1060	rBV	1010163	1340159	20.85%	2.585%
20	15.305	1171	1174	1186	rVB	403393	728090	11.33%	1.404%

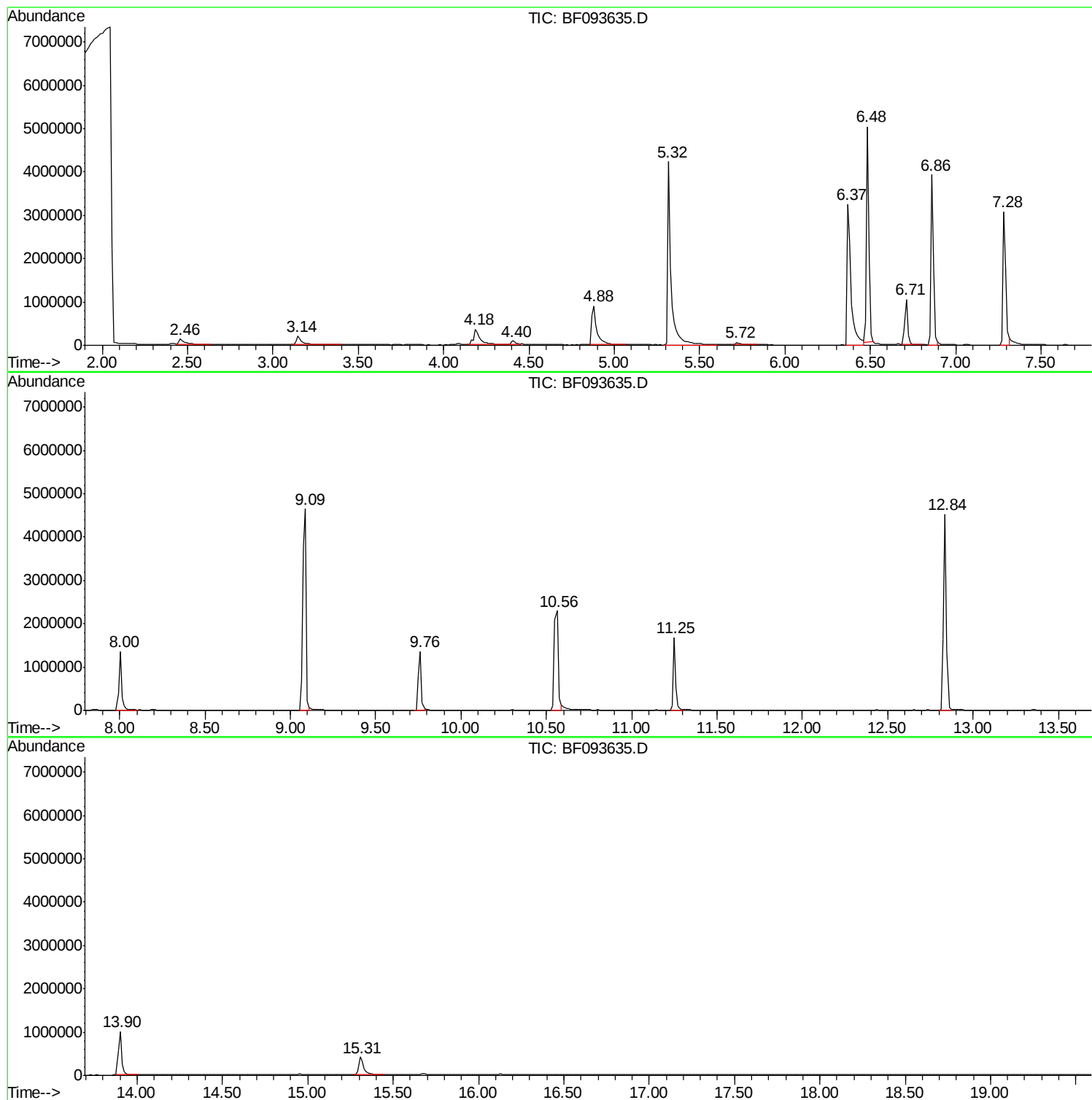
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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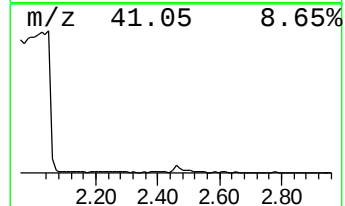
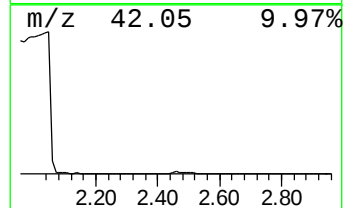
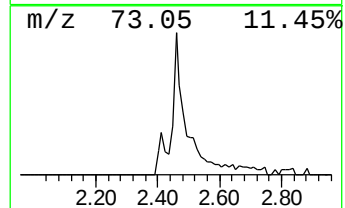
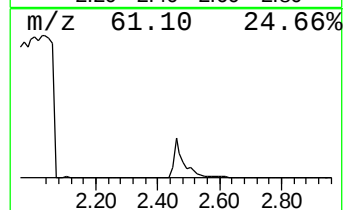
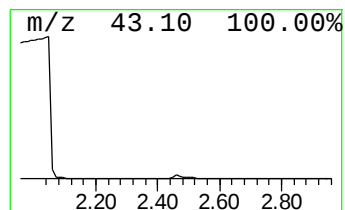
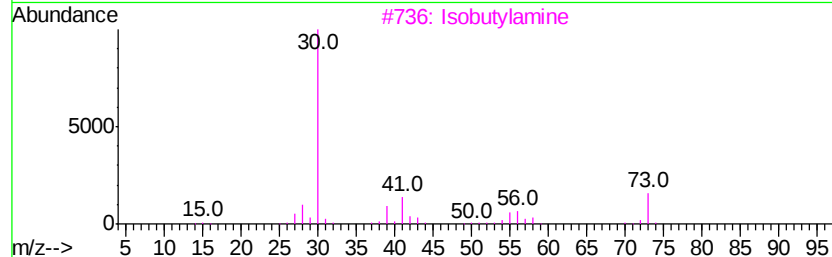
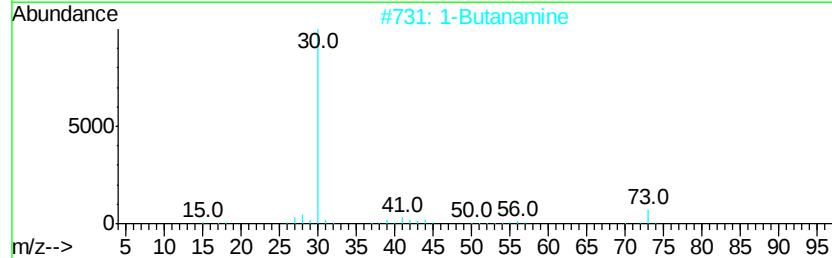
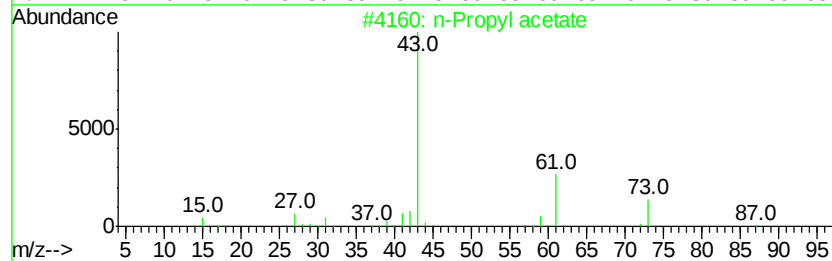
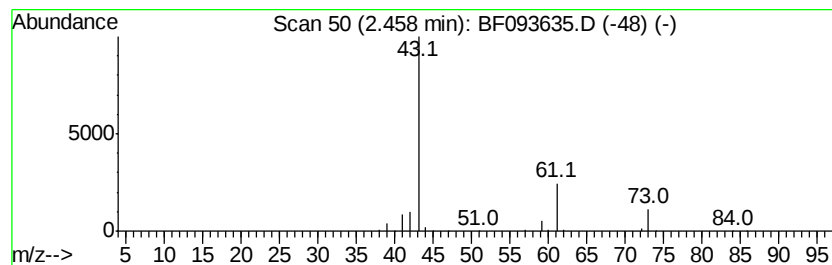
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	5.29 ng	302291	1,4-Dichlorobenzene-d4	6.71

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	5
3		Isobutylamine	73	C4H11N	000078-81-9	4
4		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4
5		Pentane	72	C5H12	000109-66-0	3



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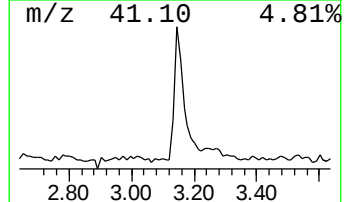
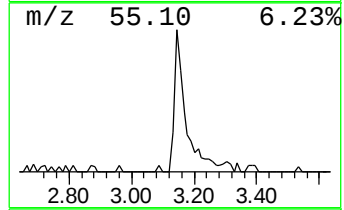
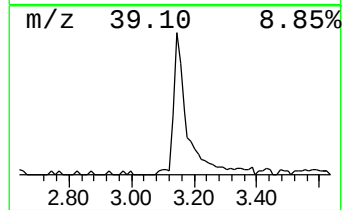
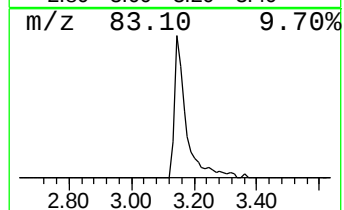
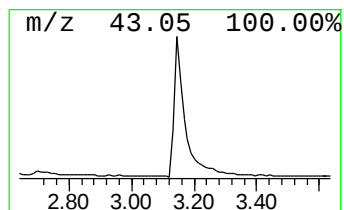
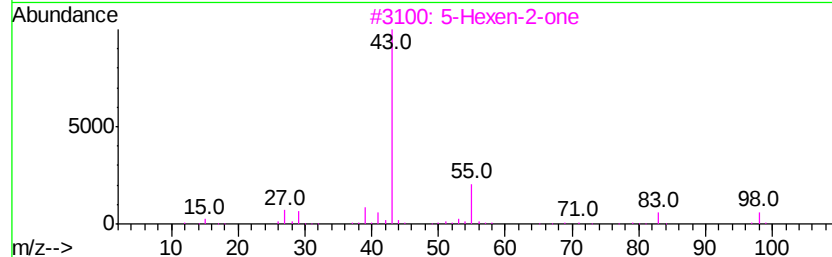
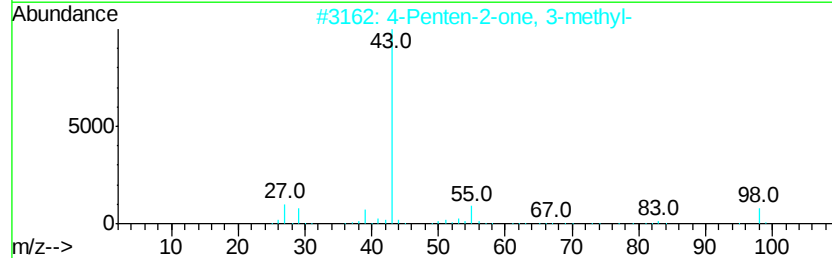
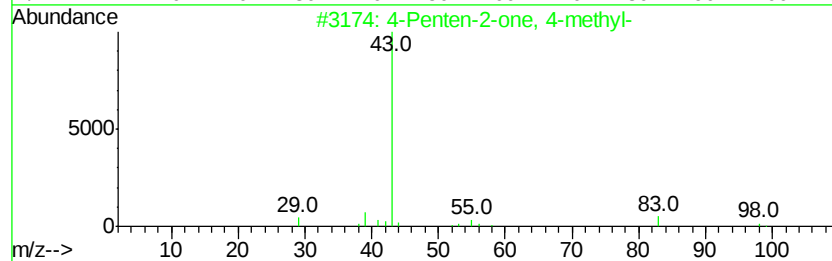
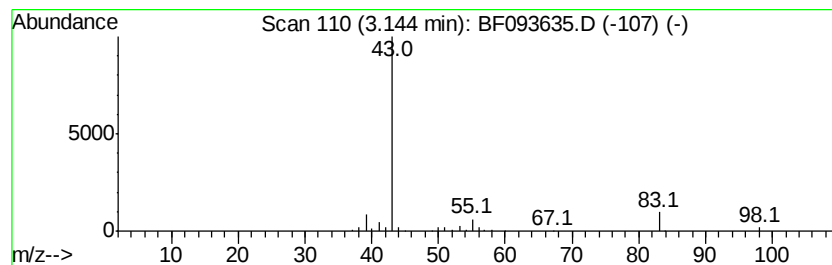
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Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	8.46 ng	483583	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	80
2		4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	53
3		5-Hexen-2-one	98	C6H10O	000109-49-9	50
4		2-Vinylethyl acetate	114	C6H10O2	001576-84-7	9
5		Pent-3-enylamine	85	C5H11N	087156-70-5	9



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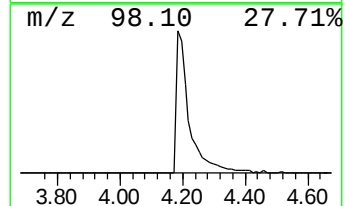
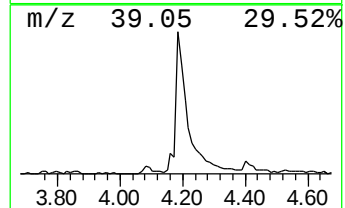
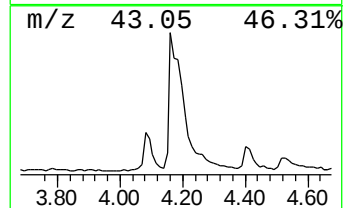
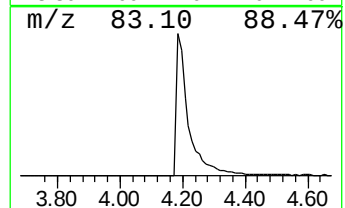
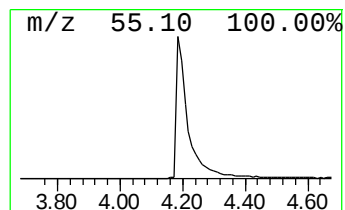
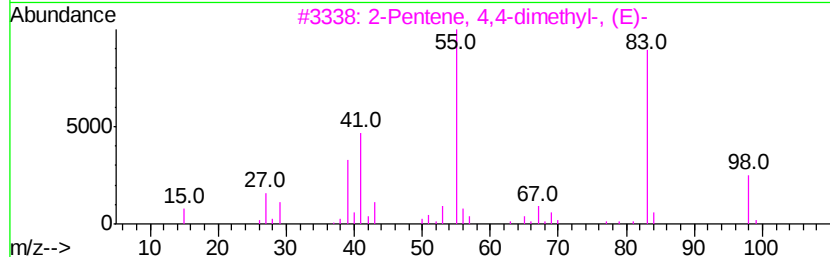
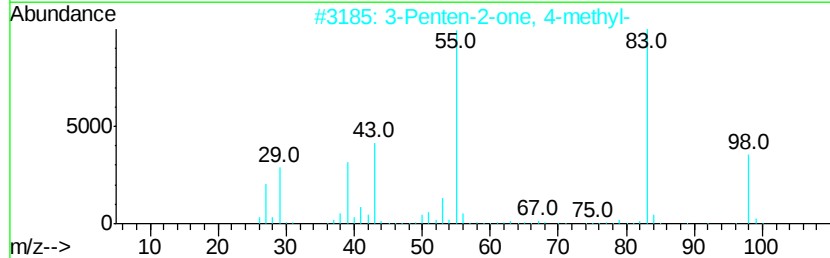
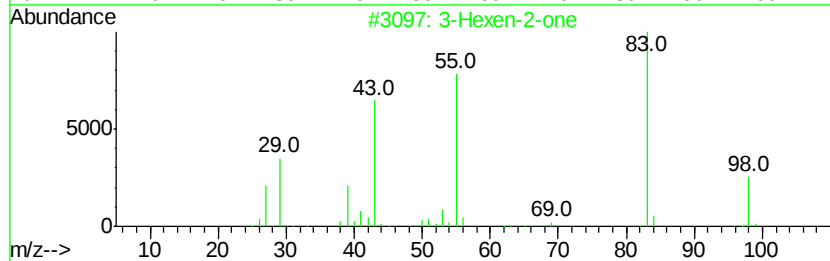
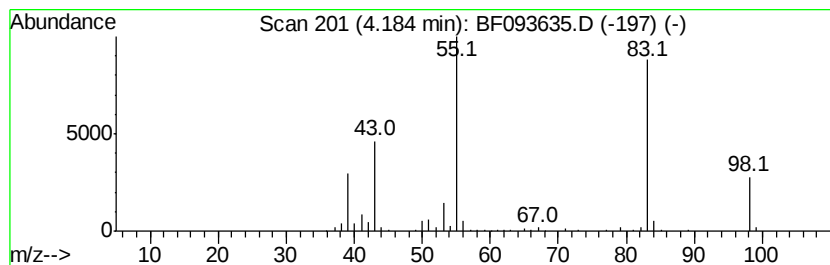
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Peak Number 3 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.18	18.28 ng	1044980	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86



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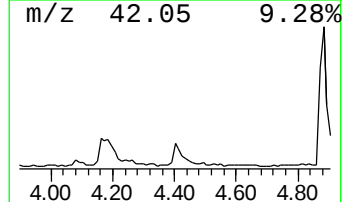
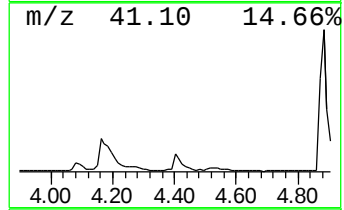
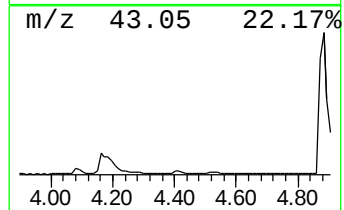
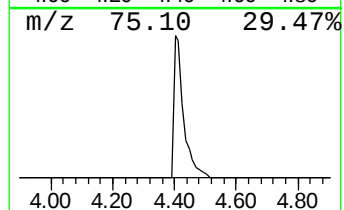
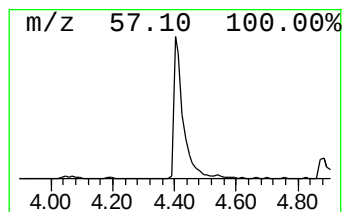
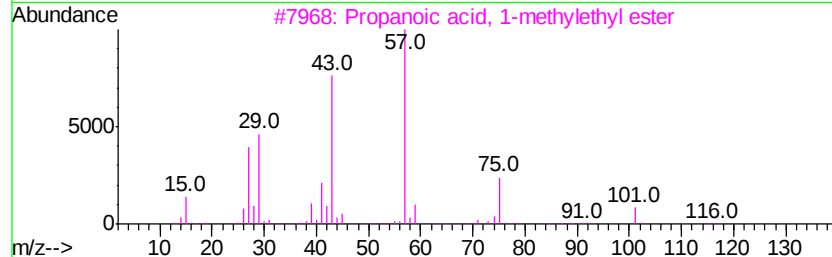
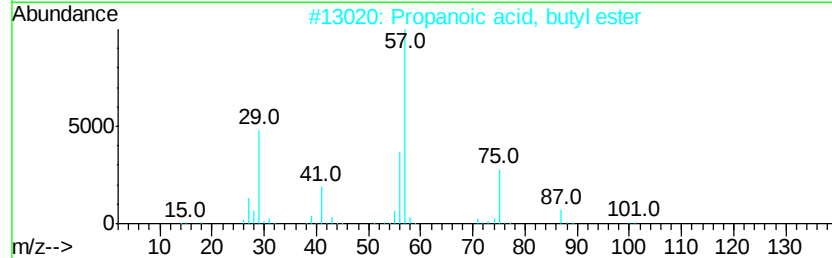
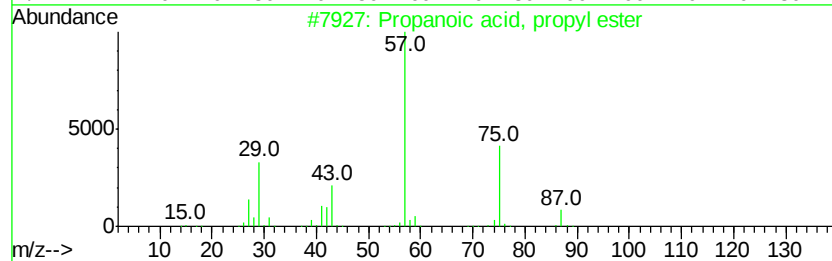
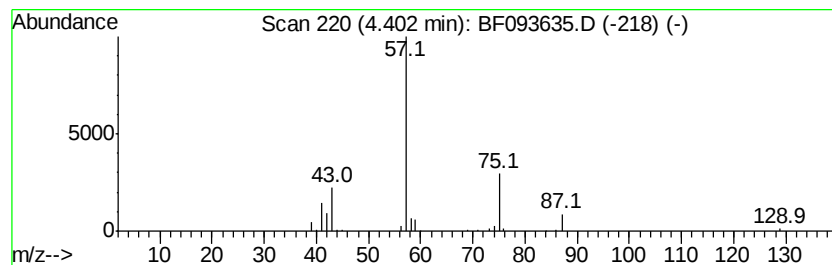
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 Propanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	2.62 ng	149689	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9
3		Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	9
4		1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	9
5		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9



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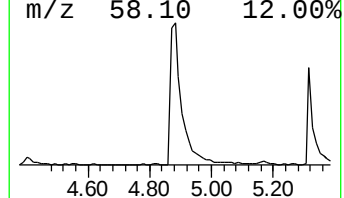
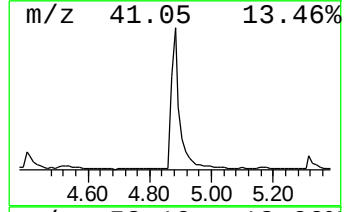
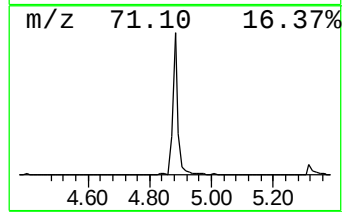
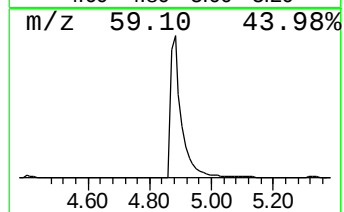
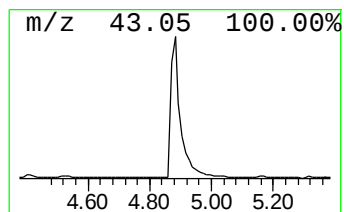
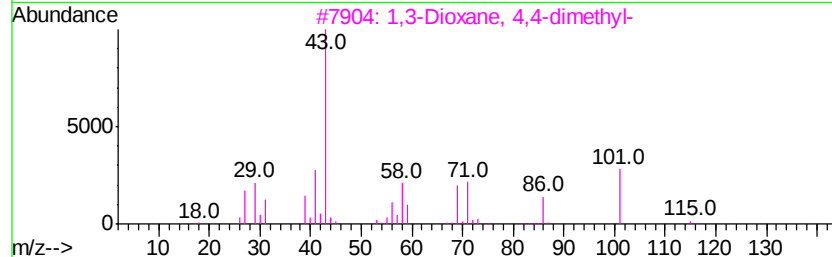
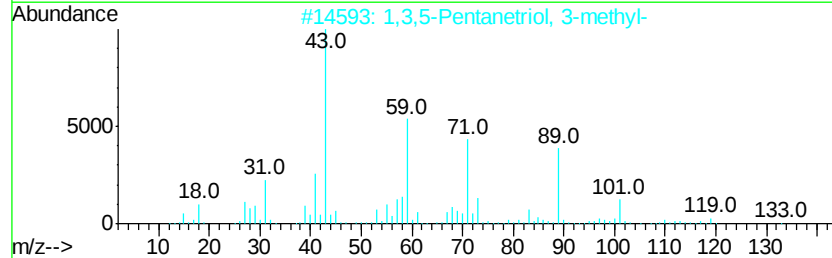
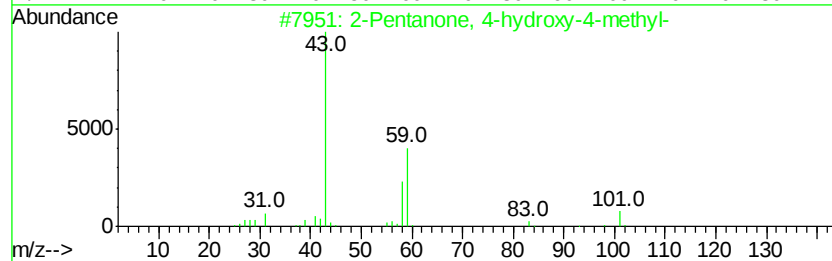
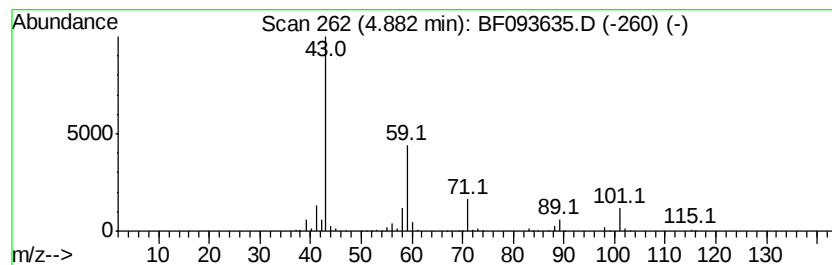
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	33.38 ng	1907730	1,4-Dichlorobenzene-d4	6.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	38
3		1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		t-Butyl nitrite	103	C4H9NO2	000540-80-7	9



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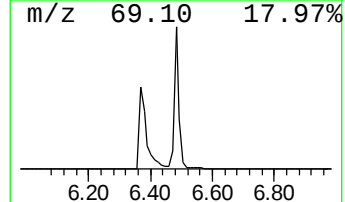
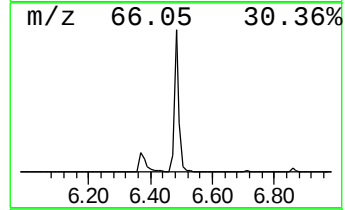
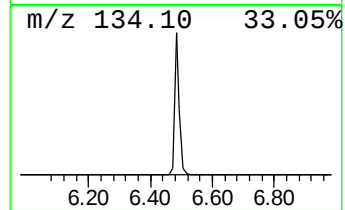
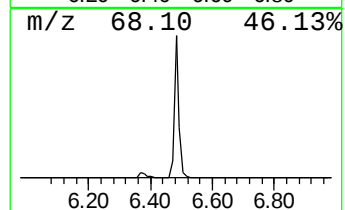
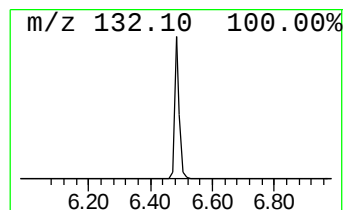
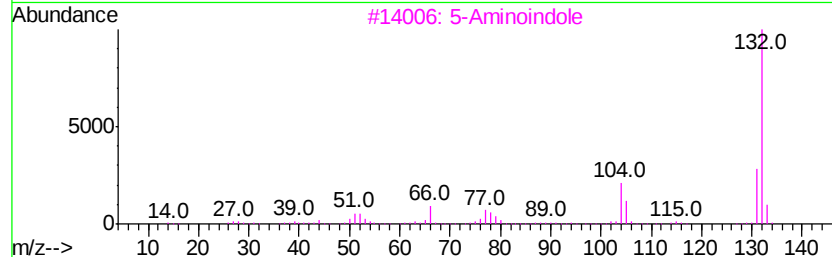
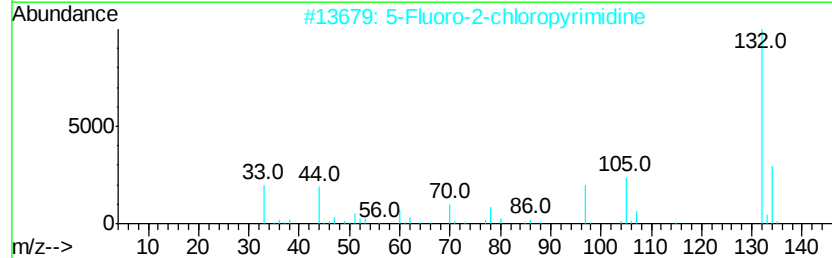
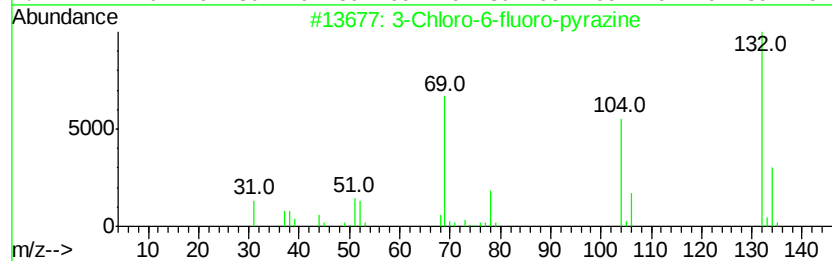
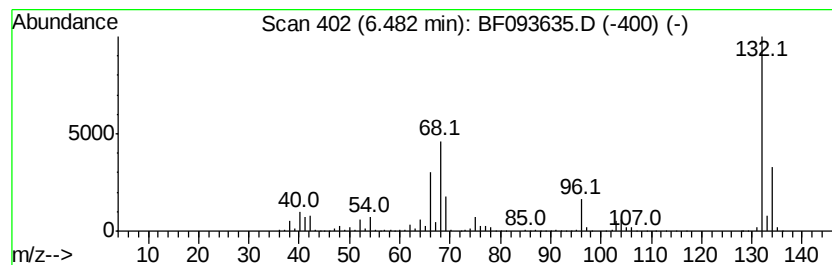
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	91.19 ng	5211790	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		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093635.D
Acq On : 14 Mar 2017 4:21
Operator : SJ/MA
Sample : I2199-27
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-105

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	5.3	ng	302291	1	6.71	1143030	20.0
4-Penten-2-one, 4...	3.14	8.5	ng	483583	1	6.71	1143030	20.0
3-Hexen-2-one	4.18	18.3	ng	1044980	1	6.71	1143030	20.0
Propanoic acid, p...	4.40	2.6	ng	149689	1	6.71	1143030	20.0
2-Pentanone, 4-hy...	4.88	33.4	ng	1907730	1	6.71	1143030	20.0
unknown6.48	6.48	91.2	ng	5211790	1	6.71	1143030	20.0