

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093642.D
 Acq On : 14 Mar 2017 7:34
 Operator : SJ/MA
 Sample : I2201-18
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-117

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-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	63	rVB	151313	332539	4.96%	0.591%
2	4.161	197	199	207	rBV	113230	200878	2.99%	0.357%
3	4.413	219	221	228	rBV	86024	179808	2.68%	0.319%
4	4.882	259	262	279	rBV	1330815	2916182	43.46%	5.180%
5	5.316	298	300	333	rBV	4186914	6556237	97.70%	11.647%
6	5.716	333	335	345	rVB	95208	168102	2.50%	0.299%
7	6.367	390	392	400	rBV	3298523	5758391	85.81%	10.229%
8	6.482	400	402	405	rVB	5124983	5493930	81.87%	9.760%
9	6.710	420	422	430	rVB	1041938	1258110	18.75%	2.235%
10	6.859	433	435	438	rBV	4238571	4443025	66.21%	7.893%
11	7.282	470	472	475	rBV	3310410	4175434	62.22%	7.417%
12	8.002	533	535	546	rBV	1377440	1707515	25.44%	3.033%
13	9.076	626	629	632	rBV	4540933	6710760	100.00%	11.921%
14	9.751	686	688	691	rBV	1366366	1856752	27.67%	3.298%
15	10.551	756	758	761	rBV2	2491282	3585682	53.43%	6.370%
16	11.248	817	819	824	rBV	1963658	1933544	28.81%	3.435%
17	12.654	940	942	944	rBV	205806	165649	2.47%	0.294%
18	12.837	955	958	961	rBV	4839327	5843277	87.07%	10.380%
19	13.351	1001	1003	1006	rBV	80963	115142	1.72%	0.205%
20	13.888	1049	1050	1059	rVB	1229113	1664507	24.80%	2.957%
21	15.305	1171	1174	1188	rVB	704048	1227048	18.28%	2.180%

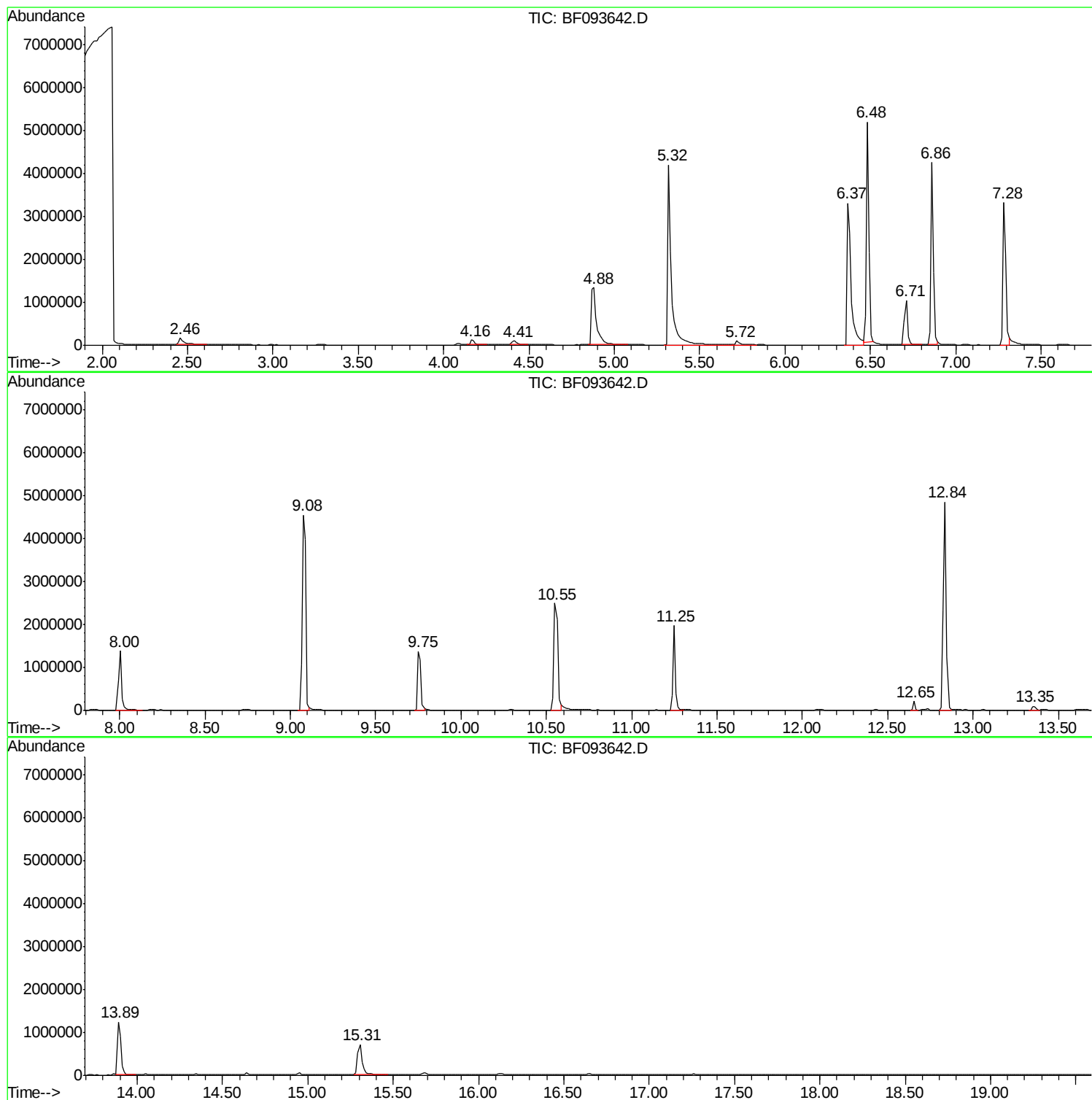
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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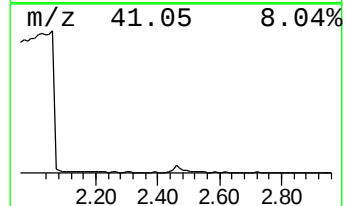
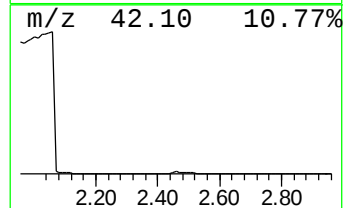
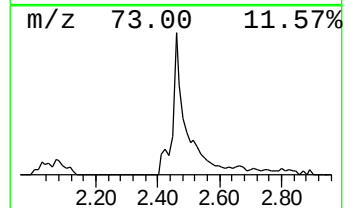
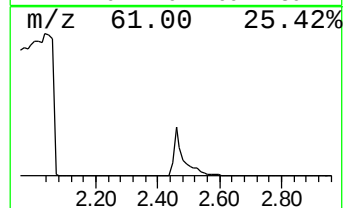
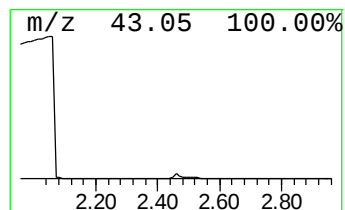
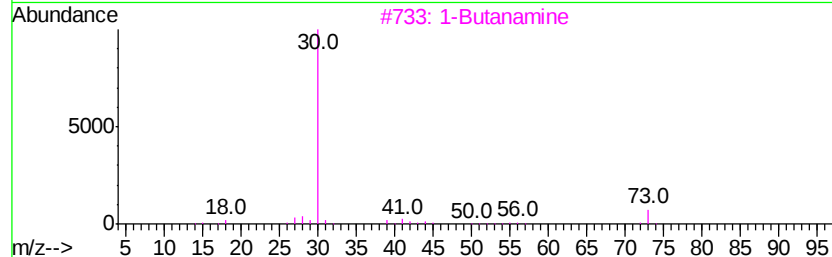
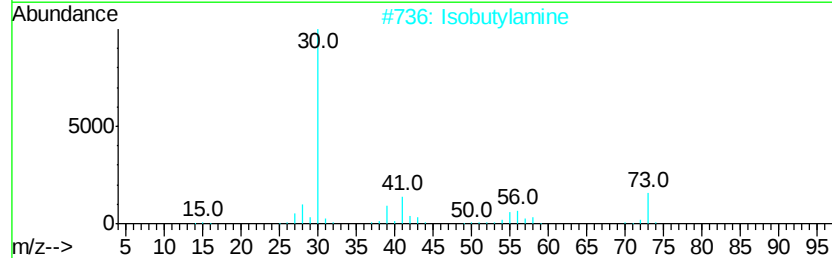
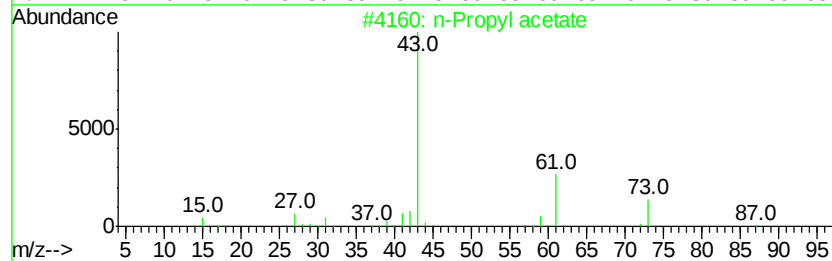
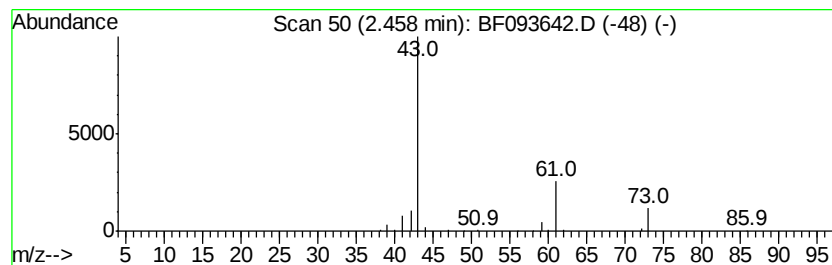
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.46	5.29 ng	332539	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		Isobutylamine	73	C4H11N	000078-81-9	5
3		1-Butanamine	73	C4H11N	000109-73-9	4
4		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4
5		Hydrogen azide	43	HN3	007782-79-8	4



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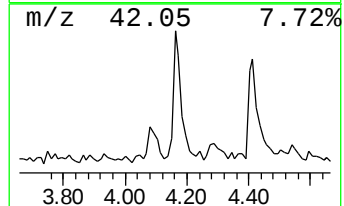
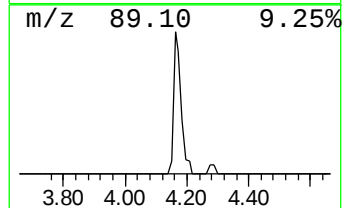
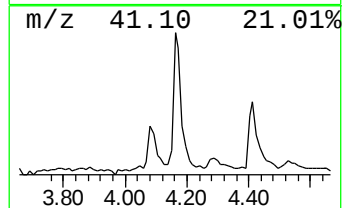
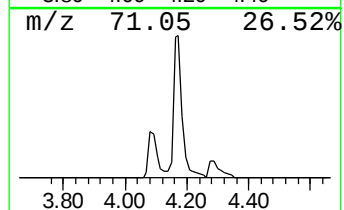
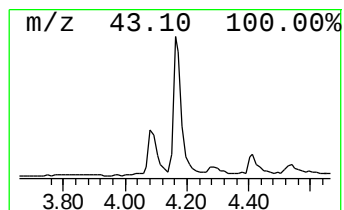
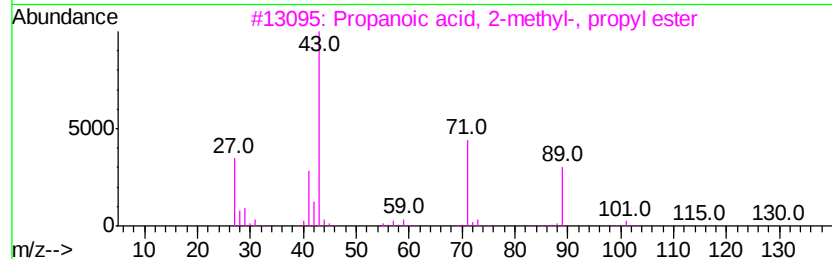
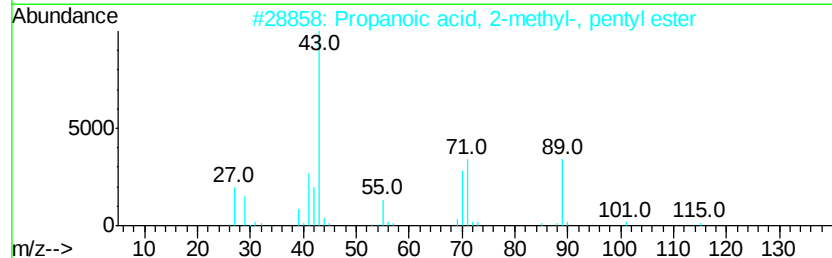
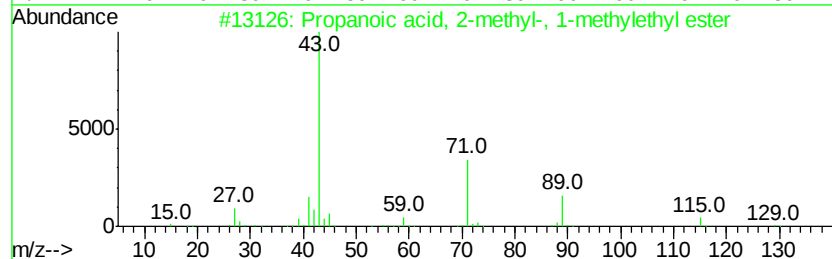
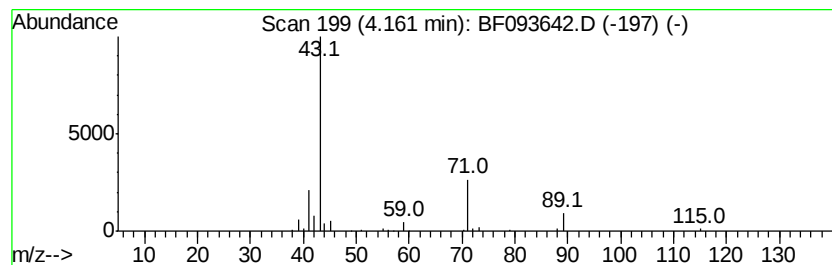
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Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	3.19 ng	200878	1,4-Dichlorobenzene-d4	6.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2		Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	33
3		Propanoic acid, 2-methyl-, propv...	130	C7H14O2	000644-49-5	25
4		N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	9
5		.beta.-Alanine	89	C3H7NO2	000107-95-9	9



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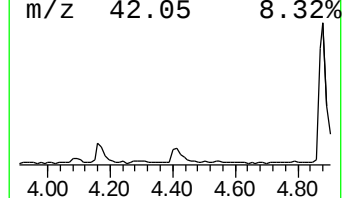
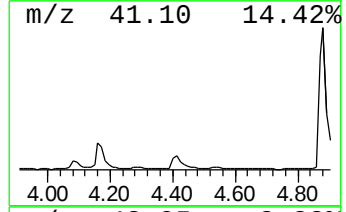
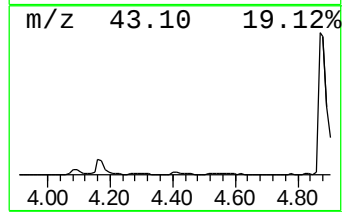
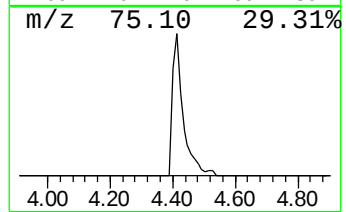
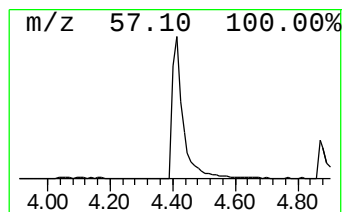
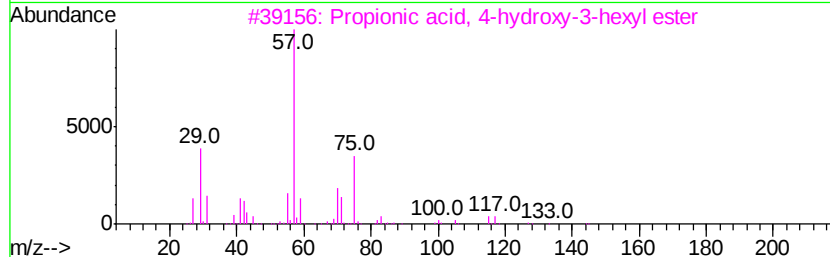
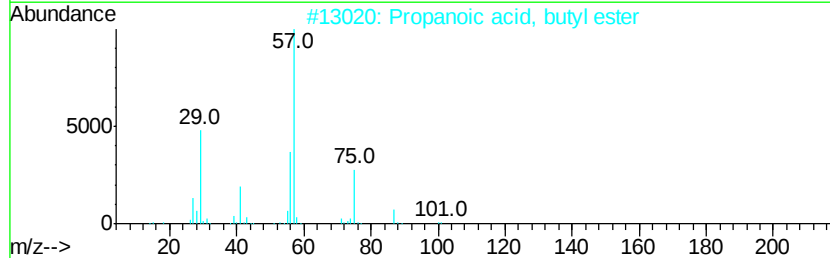
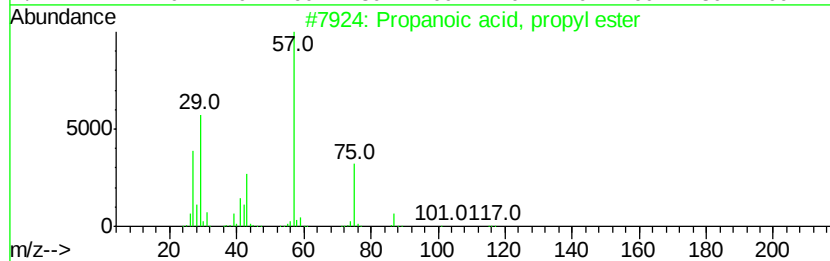
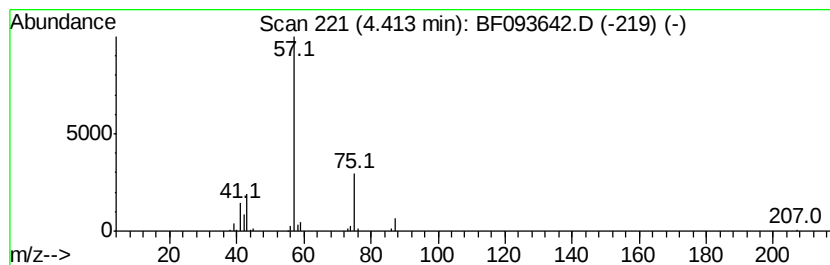
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Peak Number 3 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	2.86 ng	179808	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	78
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38
3	Propionic acid, 4-hydroxy-3-hexyl...	174	C9H18O3	1000151-16-9	9
4	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	9
5	1-Penten-3-ol	86	C5H10O	000616-25-1	7



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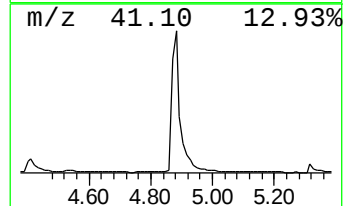
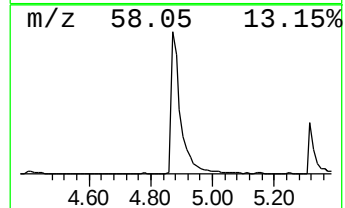
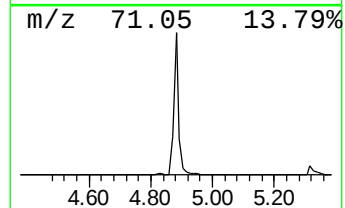
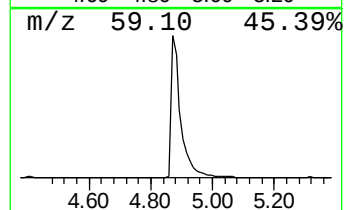
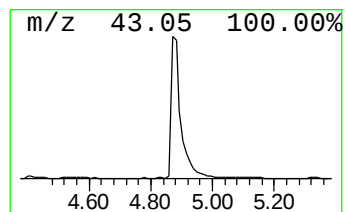
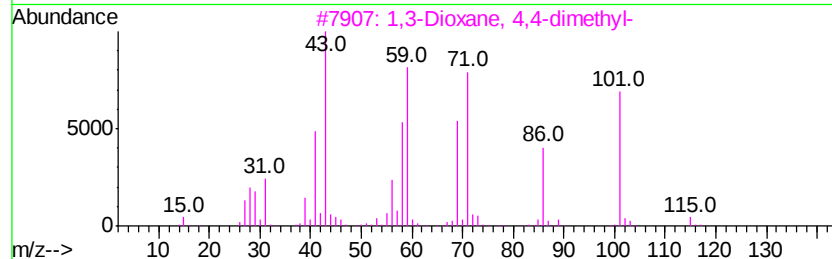
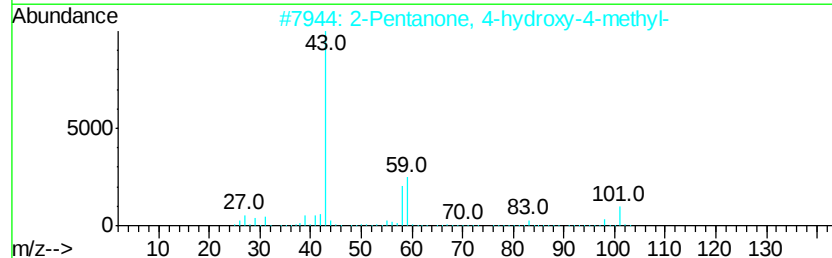
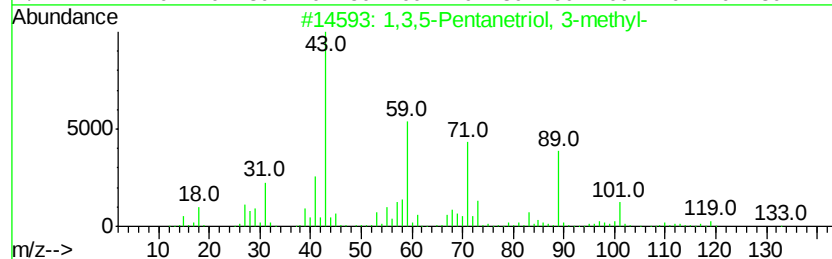
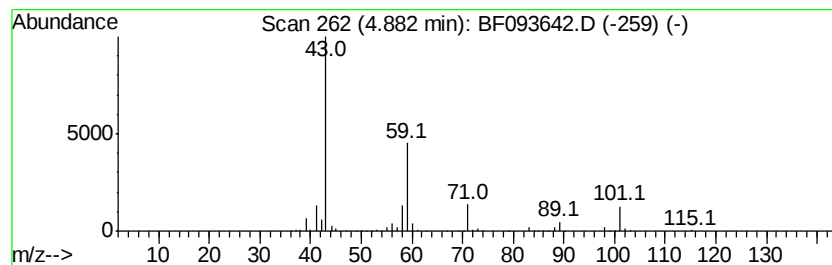
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown4.88 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	46.36 ng	2916180	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	38
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
3		1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	12
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2-Heptanone	114	C7H14O	000110-43-0	9



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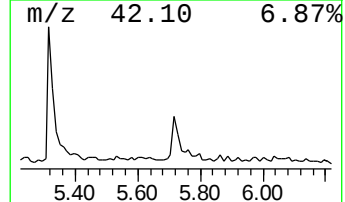
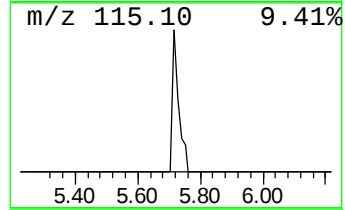
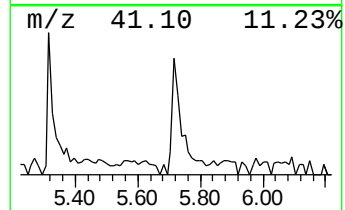
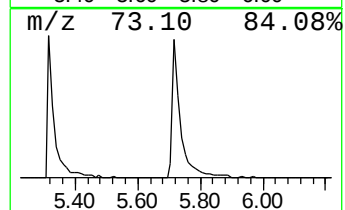
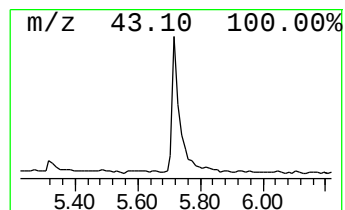
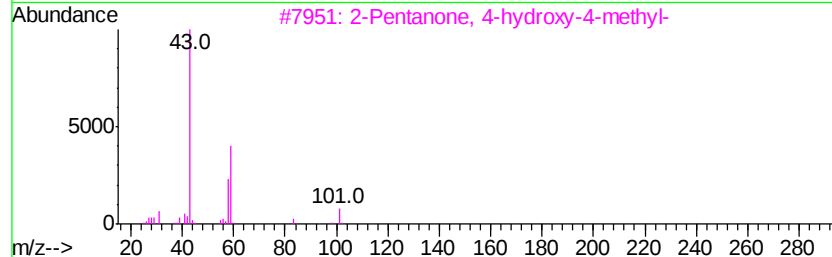
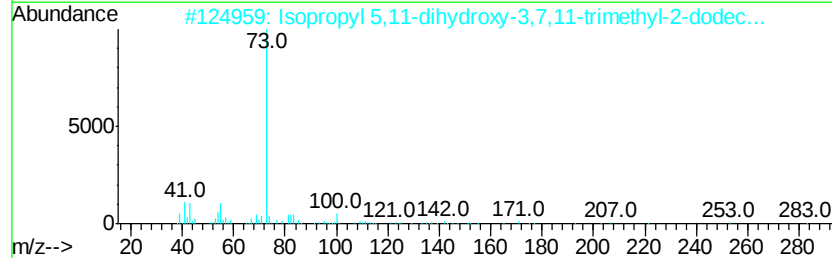
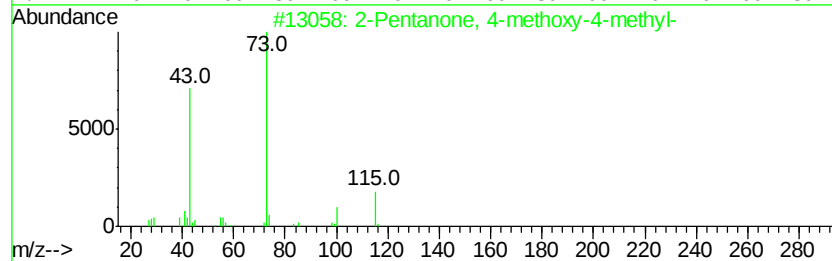
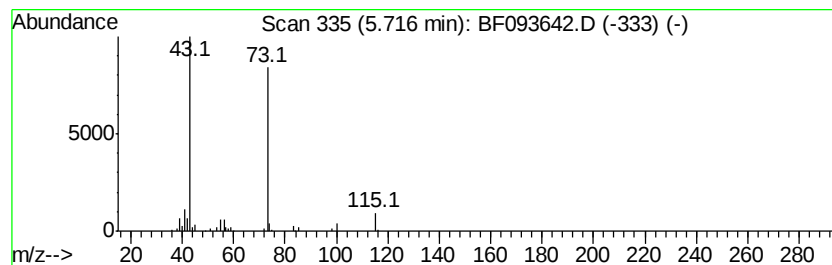
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.67 ng	168102	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		Isopropyl 5,11-dihydroxy-3,7,11-...	314	C18H34O4	1000223-34-1	17
3		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	10
4		2-Nonanone	142	C9H18O	000821-55-6	10
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10



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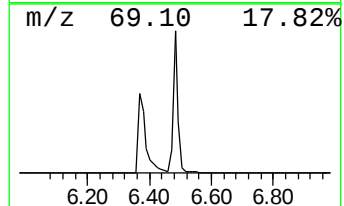
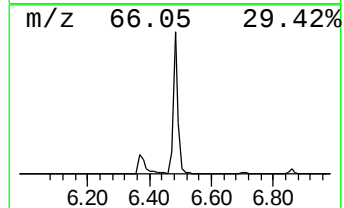
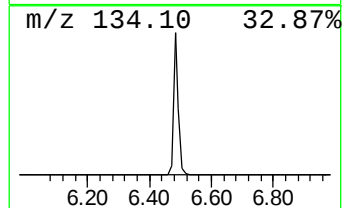
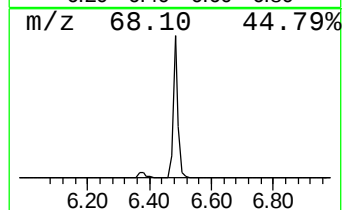
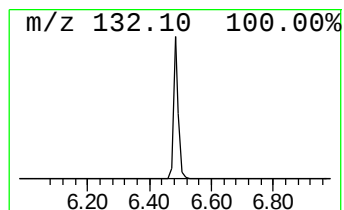
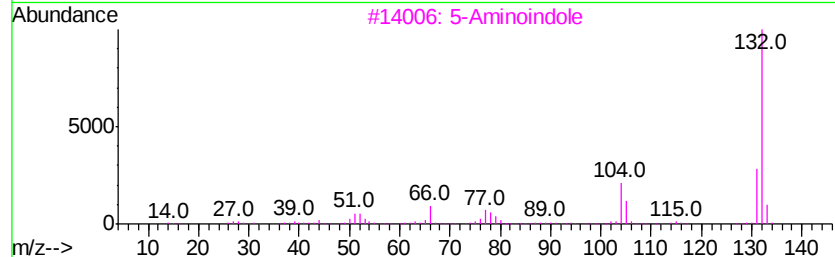
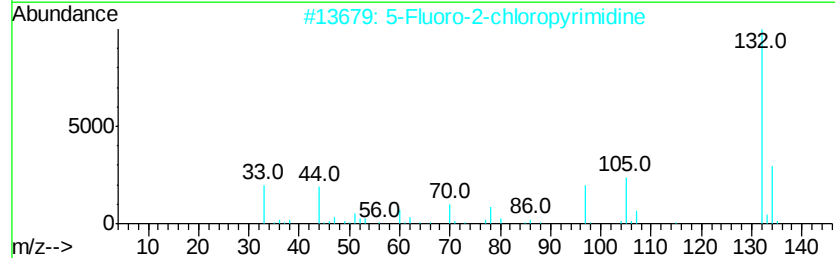
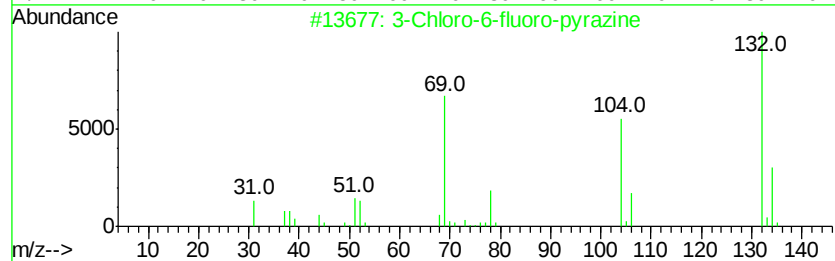
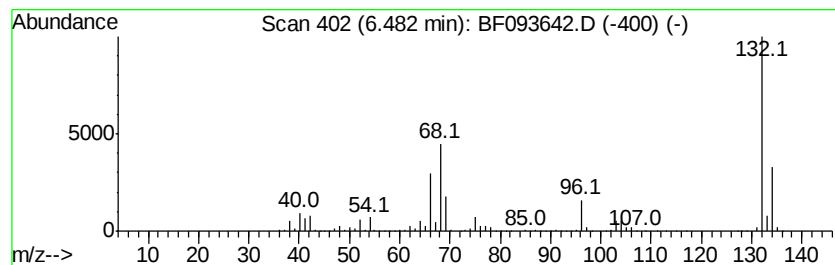
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	87.34 ng	5493930	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 : BF093642.D
Acq On : 14 Mar 2017 7:34
Operator : SJ/MA
Sample : I2201-18
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-117

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	332539	1	6.71	1258110	20.0
Propanoic acid, 2...	4.16	3.2	ng	200878	1	6.71	1258110	20.0
Propanoic acid, p...	4.41	2.9	ng	179808	1	6.71	1258110	20.0
unknown4.88	4.88	46.4	ng	2916180	1	6.71	1258110	20.0
2-Pentanone, 4-me...	5.72	2.7	ng	168102	1	6.71	1258110	20.0
unknown6.48	6.48	87.3	ng	5493930	1	6.71	1258110	20.0