

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
 Data File : BF093646.D
 Acq On : 14 Mar 2017 9:25
 Operator : SJ/MA
 Sample : I2201-22
 Misc :
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 D-123

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	2.447	47	49	61	rVB	47252	148754	2.49%	0.300%
2	4.162	197	199	206	rVB	47544	85740	1.44%	0.173%
3	4.413	219	221	231	rBV	31727	74839	1.25%	0.151%
4	4.870	259	261	278	rBV	1293757	2583111	43.24%	5.212%
5	5.316	298	300	325	rBV	4190905	5973787	100.00%	12.053%
6	5.716	333	335	349	rVB	79429	163308	2.73%	0.329%
7	6.367	390	392	400	rBV	3312697	5244780	87.80%	10.582%
8	6.482	400	402	405	rVB	4883153	5021231	84.05%	10.131%
9	6.710	420	422	429	rVB	1040876	1111238	18.60%	2.242%
10	6.859	433	435	438	rBV	3948471	4027879	67.43%	8.127%
11	7.282	470	472	488	rBV	3000659	3669471	61.43%	7.403%
12	8.002	533	535	547	rBV	1216153	1547378	25.90%	3.122%
13	9.076	627	629	632	rBV	4562865	5675983	95.01%	11.452%
14	9.751	686	688	691	rBV	1111807	1611863	26.98%	3.252%
15	10.551	756	758	761	rBV2	2396382	3123573	52.29%	6.302%
16	11.248	816	819	825	rBV	1706368	1685455	28.21%	3.401%
17	12.654	940	942	945	rBV	281481	240481	4.03%	0.485%
18	12.837	955	958	961	rBV	4657566	5105480	85.46%	10.301%
19	13.362	1001	1004	1006	rBV	151405	151643	2.54%	0.306%
20	13.900	1049	1051	1061	rBV	925888	1325107	22.18%	2.674%
21	15.306	1171	1174	1185	rBV	637792	993300	16.63%	2.004%

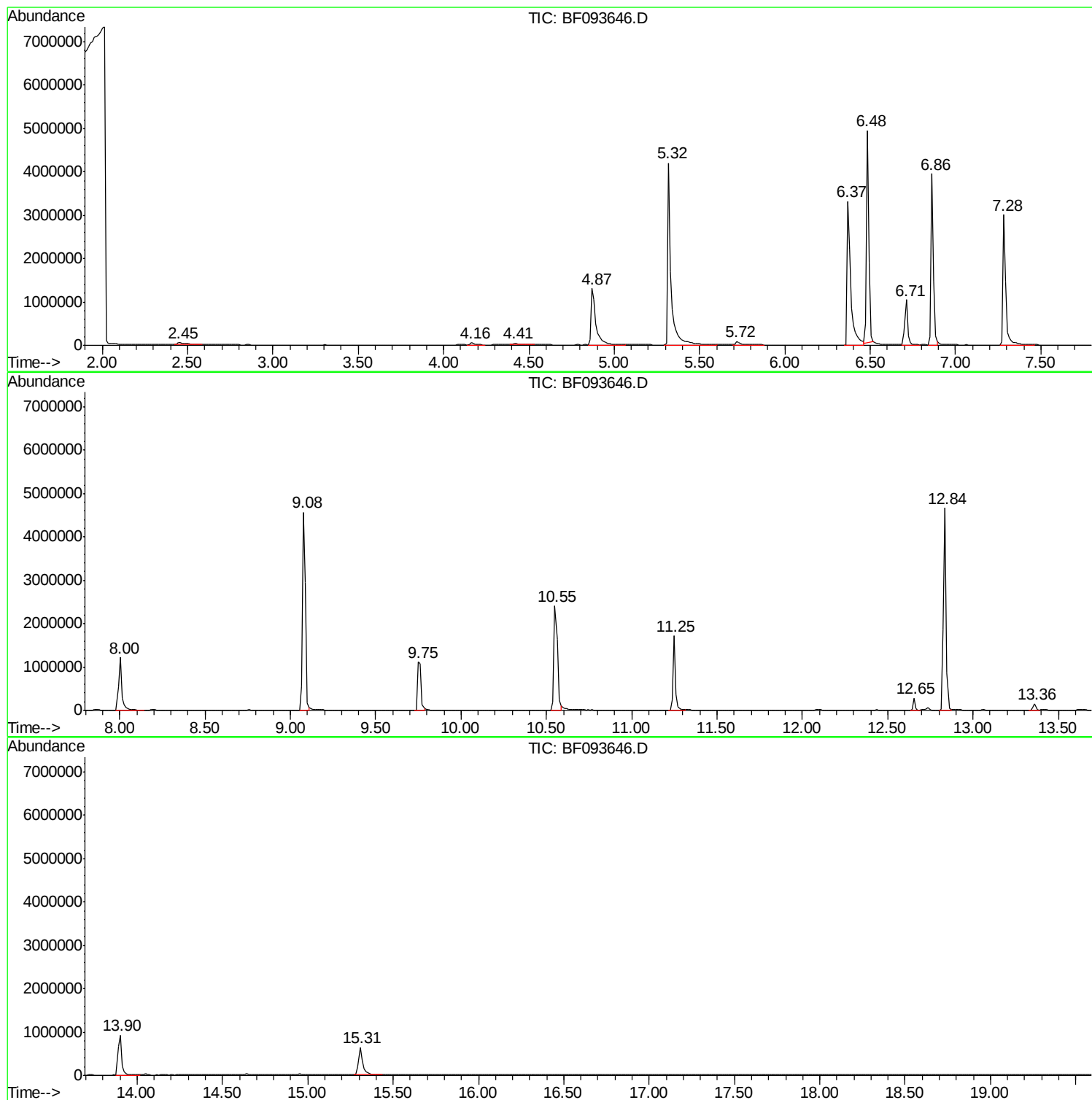
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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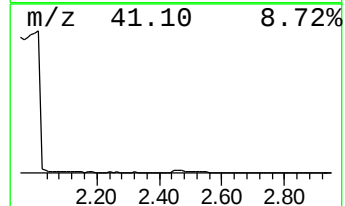
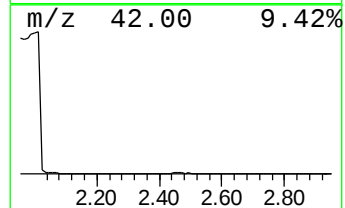
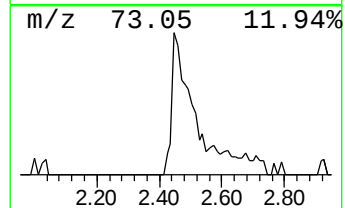
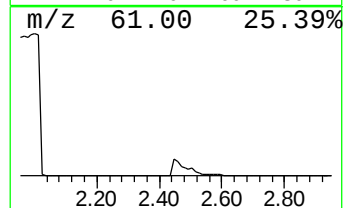
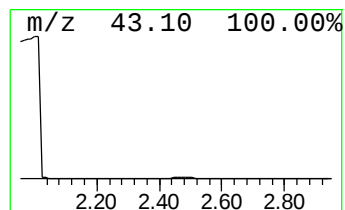
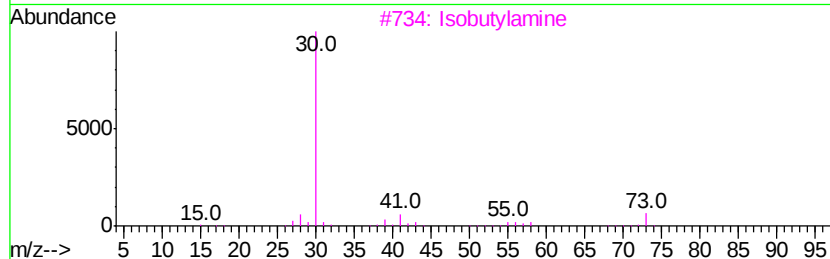
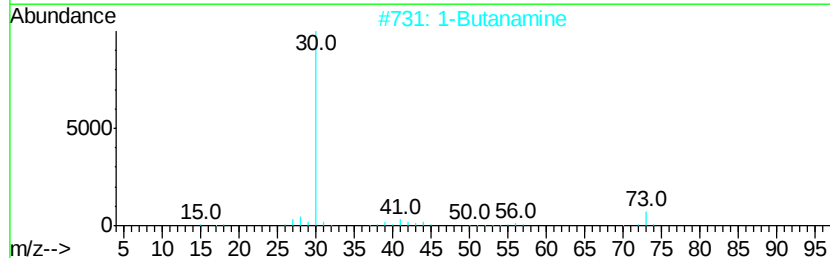
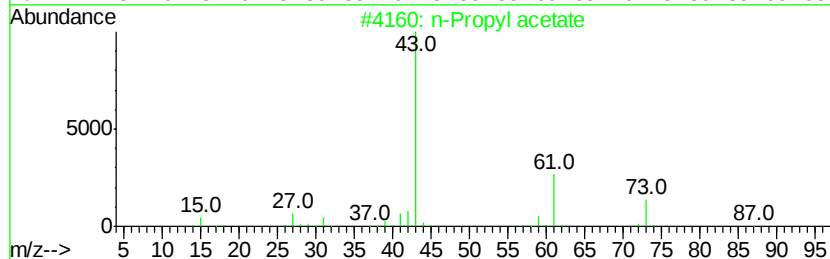
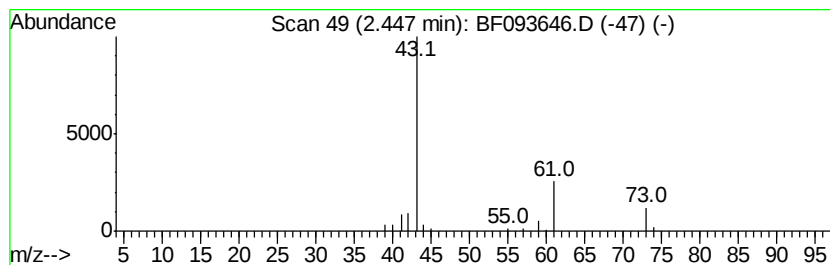
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	2.68 ng	148754	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2		1-Butanamine	73	C4H11N	000109-73-9	7
3		Isobutylamine	73	C4H11N	000078-81-9	4
4		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4
5		Acetic acid, pentyl ester	130	C7H14O2	000628-63-7	4



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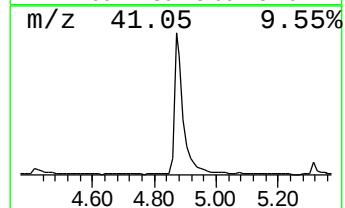
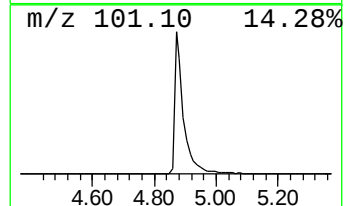
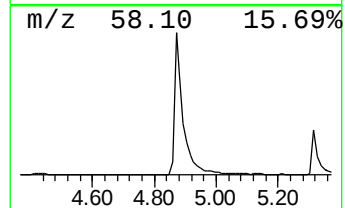
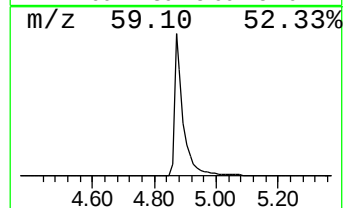
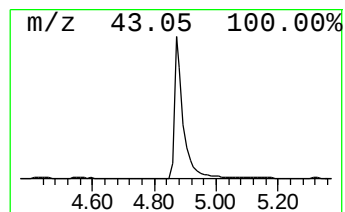
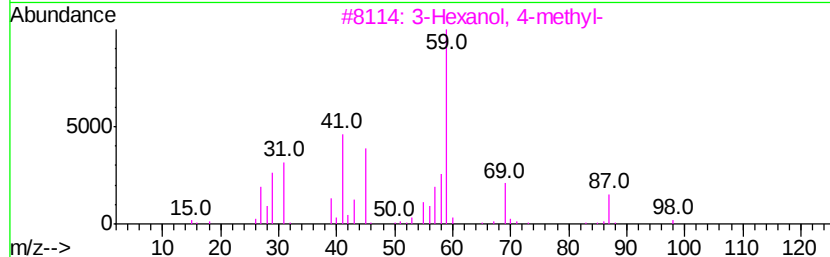
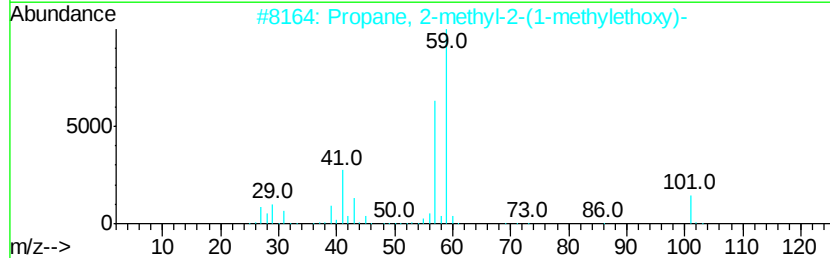
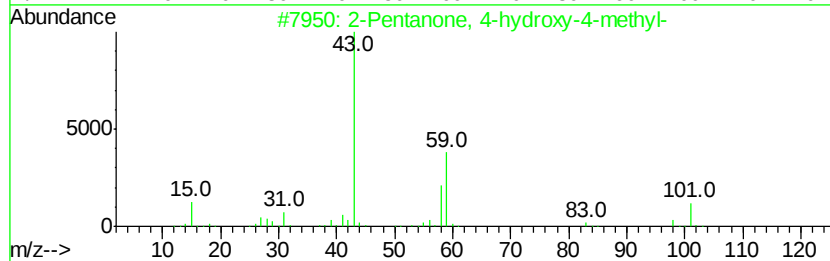
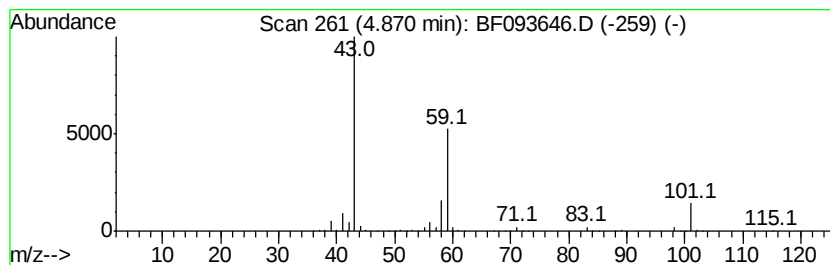
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	46.49 ng	2583110	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	53
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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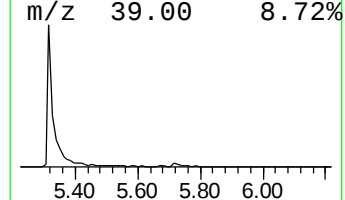
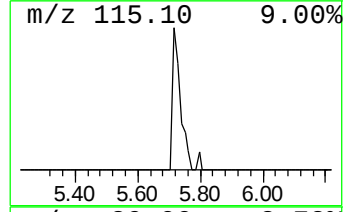
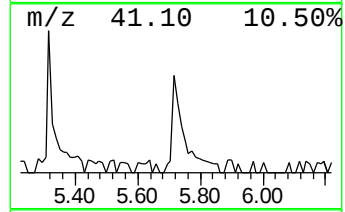
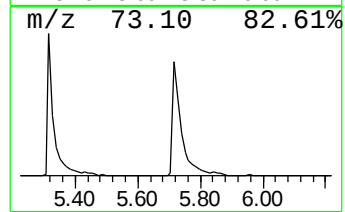
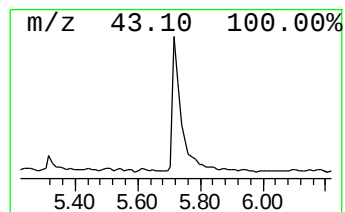
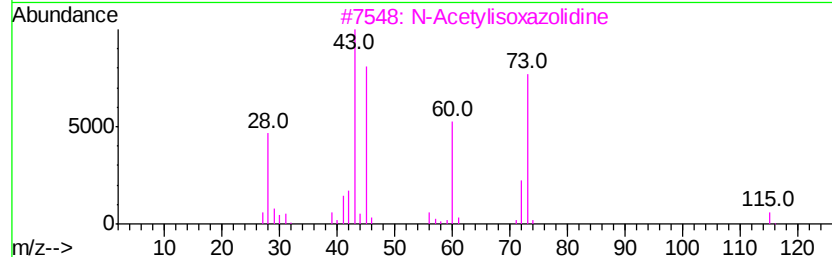
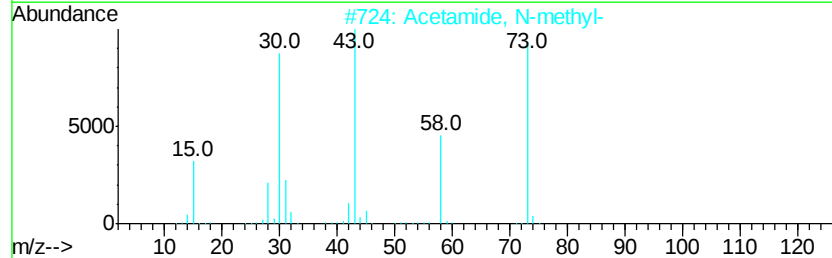
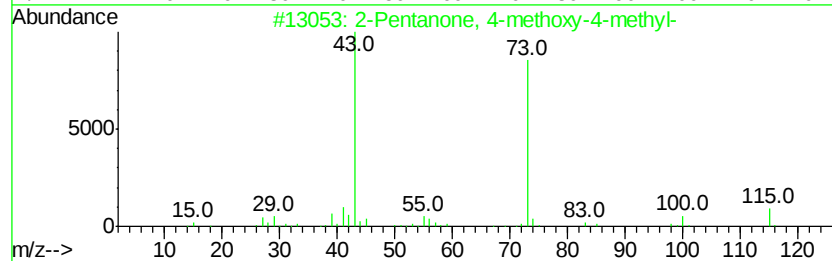
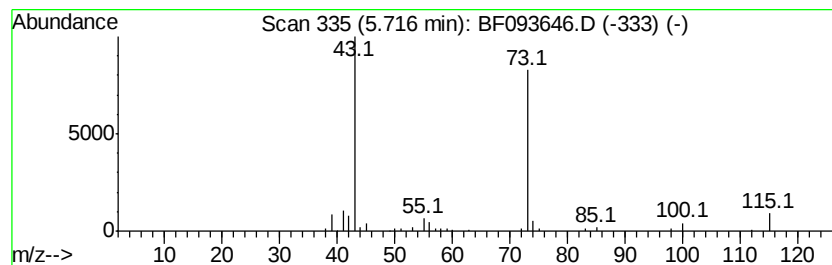
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.94 ng	163308	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	43
3		N-Acetylisoaxazolidine	115	C5H9N2O	115615-36-6	38
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	12



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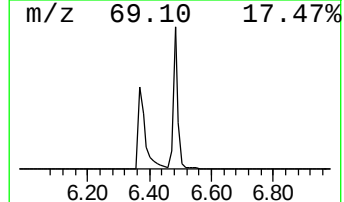
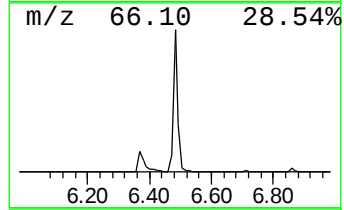
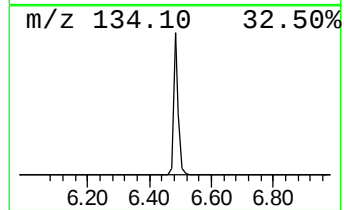
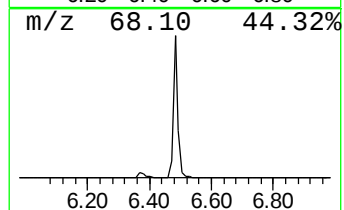
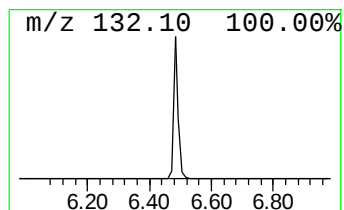
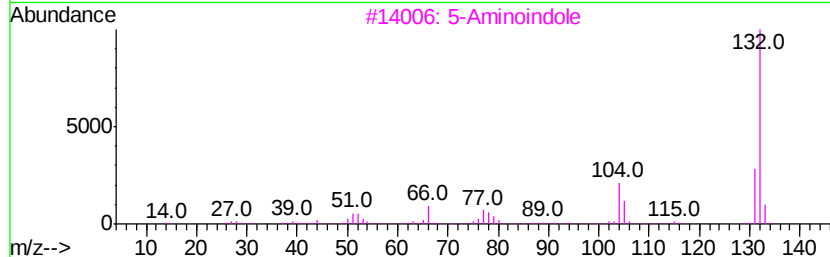
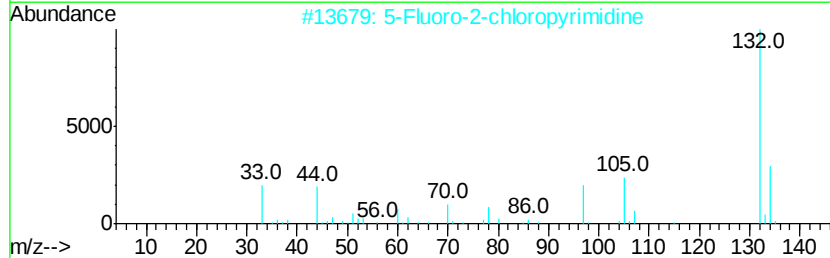
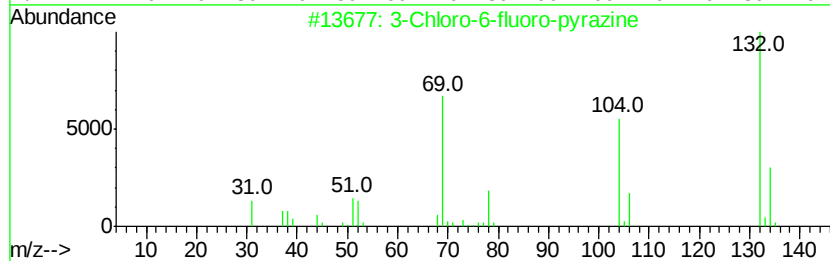
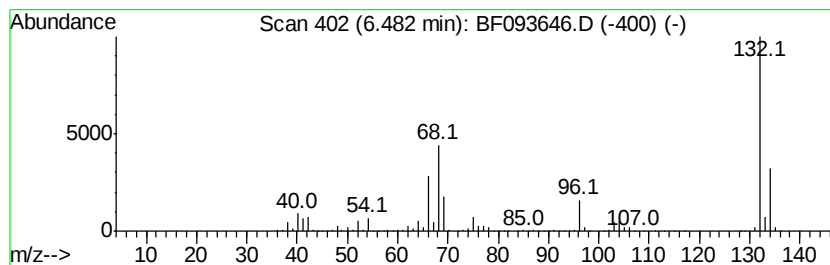
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	90.37 ng	5021230	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



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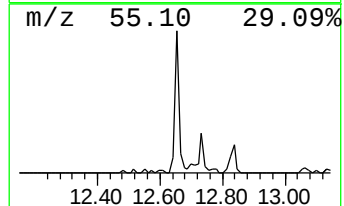
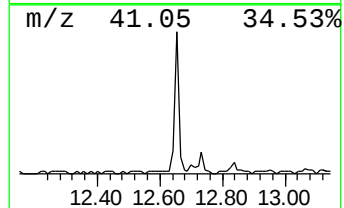
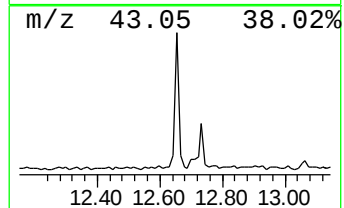
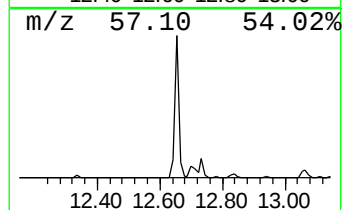
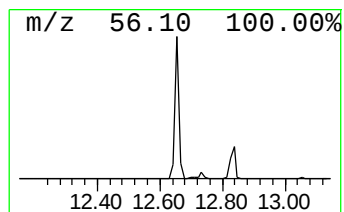
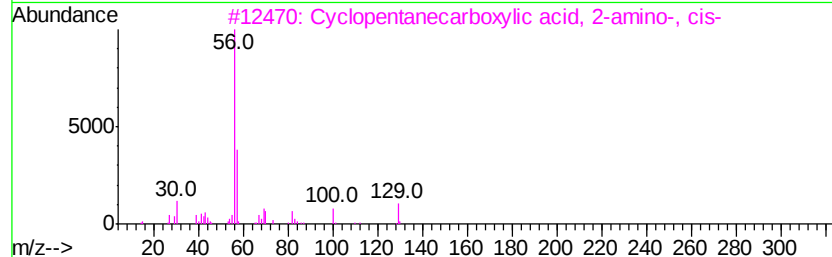
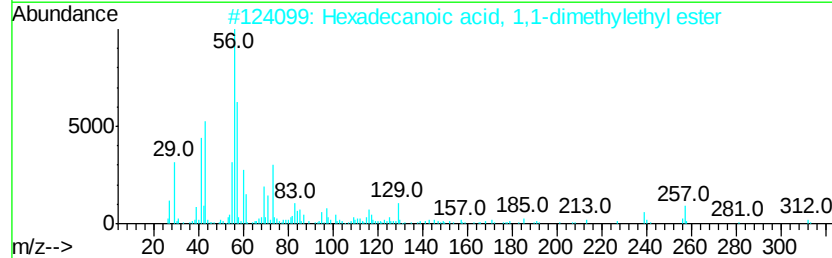
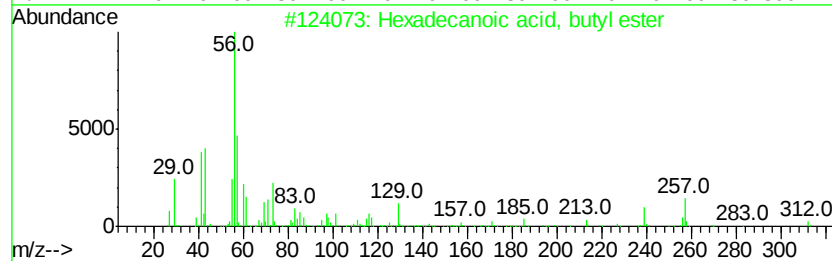
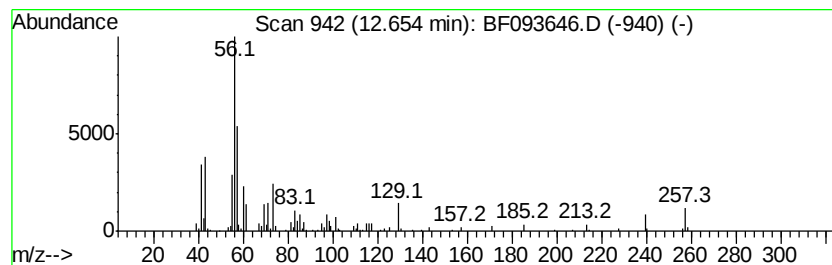
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	3.63 ng	240481	Chrysene-d12	13.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	53
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	52
3		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



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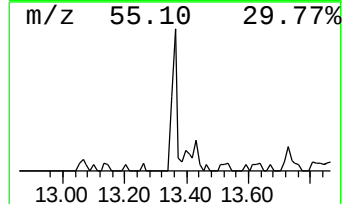
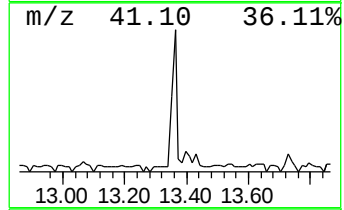
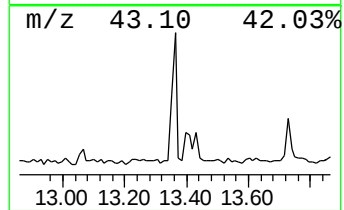
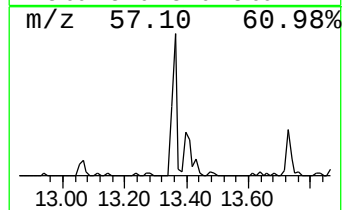
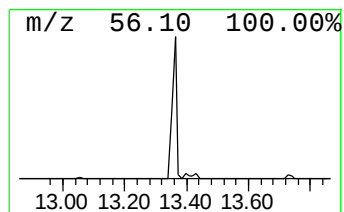
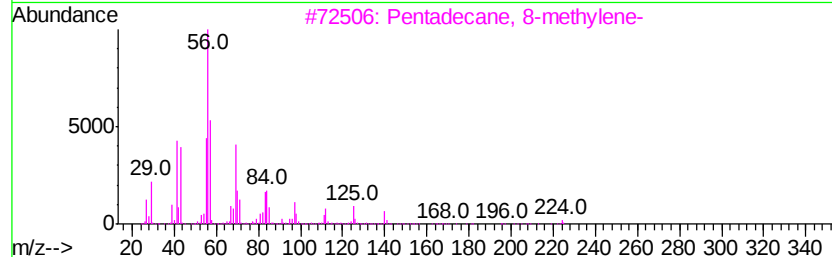
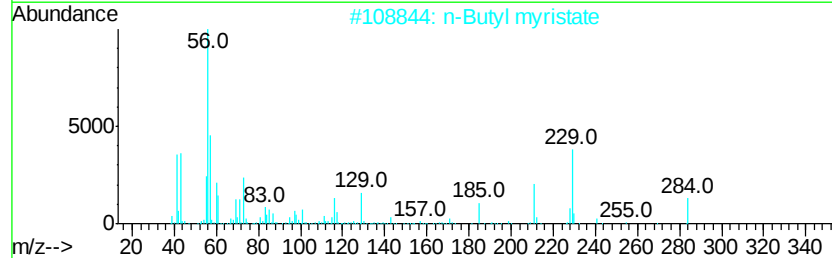
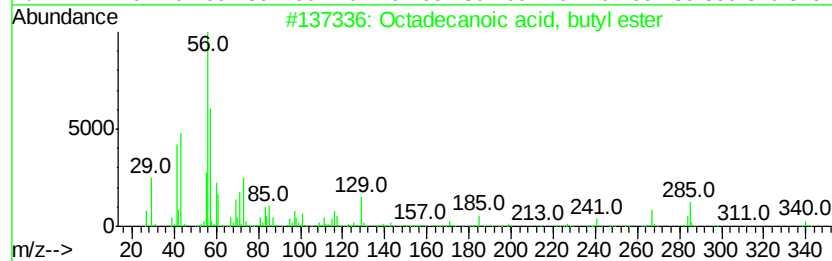
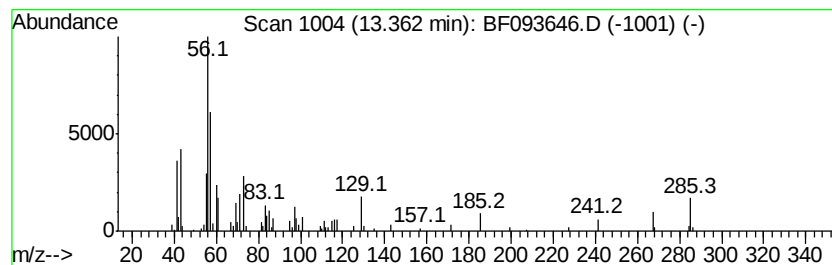
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	2.29 ng	151643	Chrysene-d12	13.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2		n-Butyl myristate	284	C18H36O2	000110-36-1	64
3		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
4		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35
5		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093646.D
Acq On : 14 Mar 2017 9:25
Operator : SJ/MA
Sample : I2201-22
Misc :
ALS Vial : 46 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D-123

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	2.45	2.7	ng	148754	1	6.71	1111240	20.0
2-Pentanone, 4-hy...	4.87	46.5	ng	2583110	1	6.71	1111240	20.0
2-Pentanone, 4-me...	5.72	2.9	ng	163308	1	6.71	1111240	20.0
unknown6.48	6.48	90.4	ng	5021230	1	6.71	1111240	20.0
Hexadecanoic acid...	12.65	3.6	ng	240481	5	13.90	1325110	20.0
Octadecanoic acid...	13.36	2.3	ng	151643	5	13.90	1325110	20.0